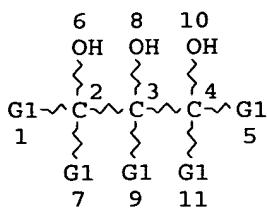


=> d que stat 125
L10 STR



VAR G1=H/D

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L15 SCR 2039

L16 SCR 2045

L19 2049 SEA FILE=REGISTRY SSS FUL L10 AND (L15 OR L16)

L20 3350 SEA FILE=HCAPLUS ABB=ON L19

L21 1971 SEA FILE=HCAPLUS ABB=ON L20 AND (?ISOTOP? OR ?LABEL?)

L22 157 SEA FILE=HCAPLUS ABB=ON L21 AND ?GLYCEROL?

L23 62 SEA FILE=HCAPLUS ABB=ON L22 AND ?SYNTHESIS?

L24 58 SEA FILE=HCAPLUS ABB=ON L23 AND (PRD<20030730 OR PD<20030730)

L25 20 SEA FILE=HCAPLUS ABB=ON L24 AND (C12 OR 12C OR C13 OR 13C)

=> d ibib abs hitstr 125 1-20

L25 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:91020 HCAPLUS

DOCUMENT NUMBER: 139:22408

TITLE: A highly efficient synthesis of [1-
13C, 18O]- and [1-13C, 2H2]-
glycerol for the elucidation of biosynthetic
pathways

AUTHOR(S): Siskos, Alexandros P.; Hill, Alison M.

CORPORATE SOURCE: Department of Chemistry, King's College London,
London, WC2R 2LS, UKSOURCE: Tetrahedron Letters (2003), 44(4), 789-792
CODEN: TELEAY; ISSN: 0040-4039

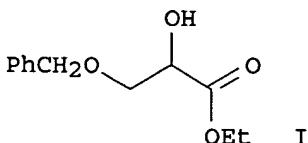
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:22408

GI



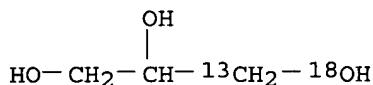
AB Labeled glycerol is a widely used biochem. probe to investigate biosynthetic pathways. A highly efficient synthesis of [1-13C, 18O]- and [1-13C, 2H2]-glycerol is described in which the 13C label is introduced using cyanide. The 18O label was introduced by a Pinner synthesis and reduction of I allowed incorporation of the 2H labels.

IT 474967-29-8P, 1,2,3-Propanetriol-1-13C-1-18O
537013-33-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of [1-13C, 18O]- and [1-13C,
2H2]-glycerol to be used in for the elucidation of
biosynthetic pathways)

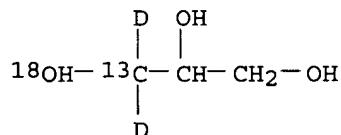
RN 474967-29-8 HCPLUS

CN 1,2,3-Propanetriol-1-13C-1-18O (9CI) (CA INDEX NAME)



RN 537013-33-5 HCPLUS

CN 1,2,3-Propane-1,1-d2-triol-1-13C-1-18O (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 20 HCPLUS COPYRIGHT 2006 ACS on STM

ACCESSION NUMBER: 2002:174867 HCPLUS

DOCUMENT NUMBER: 137:348975

TITLE: Elucidation of soraphen A biosynthesis using 2H, 13C and 18O labelled precursors

AUTHOR(S): Hill, Alison M.; Siskos, Alexandros P.; Harris, Jonathan P.

CORPORATE SOURCE: Department of Chemistry, King's College London, Strand, London, WC2R 2LS, UK

SOURCE: Synthesis and Applications of Isotopically Labelled Compounds, Proceedings of the International Symposium, 7th, Dresden, Germany, June 18-22, 2000 (2001***) , Meeting Date 2000, 626-630. Editor(s): Pleiss, Ulrich; Voges, Rolf. John Wiley & Sons Ltd.: Chichester, UK.

CODEN: 69CIJC; ISBN: 0-471-49501-8

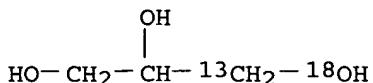
DOCUMENT TYPE: Conference

LANGUAGE: English

AB Soraphen A is a potent broad spectrum antifungal produced by the myxobacterium Sorangium cellulosum So ce26. Expts. focusing on the ***biosynthesis of soraphen A using 2H, 13C and 18O labeled precursors are discussed. The immediate precursor for the vicinal hydroxy groups in soraphen A is probably a hydroxylated extender

unit such as methoxy- or hydroxymalonate. Carboxylation of a C2 precursor, e.g., glycolate and methoxyacetate, to produce the extender unit does not appear to occur. This indicates that the C3 starting material **glycerol** is not broken down into a C2 unit such as glycine to produce the extender unit, but is instead converted to glycerate and oxidized to give the extender unit.

IT 474967-29-8, 1,2,3-Propanetriol-1-13C-1-18O
 RL: BCP (Biochemical process); RCT (Reactant); BIOL (Biological study);
 PROC (Process); RACT (Reactant or reagent)
 (soraphen A biosynthesis using labeled precursors)
 RN 474967-29-8 HCAPLUS
 CN 1,2,3-Propanetriol-1-13C-1-18O (9CI) (CA INDEX NAME)

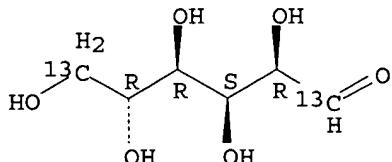


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2001:750717 HCAPLUS
 DOCUMENT NUMBER: 136:98602
 TITLE: An integrated 2H and 13C NMR study of gluconeogenesis and TCA cycle flux in humans
 AUTHOR(S): Jones, John G.; Solomon, Michael A.; Cole, Suzanne M.; Sherry, A. Dean; Malloy, Craig R.
 CORPORATE SOURCE: Department of Radiology, University of Texas Southwestern Medical Center, Dallas, TX, 75235, USA
 SOURCE: American Journal of Physiology (2001), 281(4, Pt. 1), E848-E856
 CODEN: AJPHAP; ISSN: 0002-9513
 PUBLISHER: American Physiological Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Hepatic glucose synthesis from glycogen, glycerol, and the tricarboxylic acid (TCA) cycle was measured in 5 overnight-fasted subjects by 1H, 2H, and 13C NMR anal. of blood glucose, urinary acetaminophen glucuronide, and urinary phenylacetylglutamine after administration of [1,6-13C2]glucose, 2H2O, and [U-13C3]propionate. This combination of tracers allows 3 sep. elements of hepatic glucose production (GP) to be probed simultaneously in a single study: (1) endogenous GP, (2) the contribution of glycogen, phosphoenolpyruvate (PEP), and glycerol to GP, and (3) flux through PEP carboxykinase, pyruvate recycling, and the TCA cycle. Isotope-dilution measurements of [1,6-13C2]glucose by 1H and 13C NMR indicated that GP in 16-h-fasted humans was $10.7 \pm 0.9 \mu\text{mol} \cdot \text{kg}^{-1} \cdot \text{min}^{-1}$. 2H NMR spectra of monoacetone glucose (derived from plasma glucose) provided the relative 2H enrichment at glucose H-2, H-5, and H-6S, which, in turn, reflects the contribution of glycogen, PEP, and glycerol to total GP (5.5 ± 0.7 , 4.8 ± 1.0 , and $0.4 \pm 0.3 \mu\text{mol} \cdot \text{kg}^{-1} \cdot \text{min}^{-1}$, resp.). Interestingly, 13C NMR isotopomer anal. of phenylacetylglutamine and acetaminophen glucuronide reported different values for PEP carboxykinase flux (68.8 ± 9.8 vs. $37.5 \pm 7.9 \mu\text{mol} \cdot \text{kg}^{-1} \cdot \text{min}^{-1}$), PEP recycling flux (59.1 ± 9.8 vs. $27.8 \pm 6.8 \mu\text{mol} \cdot \text{kg}^{-1} \cdot \text{min}^{-1}$), and TCA cycle flux (10.9 ± 1.4 vs. $5.4 \pm 1.4 \mu\text{mol} \cdot \text{kg}^{-1} \cdot \text{min}^{-1}$). These differences may reflect zonation

of propionate metabolism in the liver.
 IT 201741-04-0, D-Glucose-1,6-13C2
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);
 ANST (Analytical study); BIOL (Biological study); USES (Uses)
 (integrated 2H and 13C NMR study of gluconeogenesis and TCA
 cycle flux in humans)
 RN 201741-04-0 HCAPLUS
 CN D-Glucose-1,6-13C2 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2000:128248 HCAPLUS
 DOCUMENT NUMBER: 132:291497
 TITLE: Metabolism of [1,3-13C]glycerol
 -1,2,3-tris(methylsuccinate) and glycerol
 -1,2,3-tris(methyl[2,3-13C]succinate) in rat
 hepatocytes
 AUTHOR(S): Malaisse, Willy J.; Ladriere, Laurence; Verbruggen,
 Ingrid; Grue-Sorenson, Gunnar; Bjorkling, Fredrik;
 Willem, Rudolph
 CORPORATE SOURCE: Laboratory of Experimental Medicine, Brussels Free
 University, Brussels, B-1070, Belg.
 SOURCE: Metabolism, Clinical and Experimental (2000
), 49(2), 178-185
 CODEN: METAAJ; ISSN: 0026-0495
 PUBLISHER: W. B. Saunders Co.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Hepatocytes prepared from overnight-fasted rats were incubated for 120 min
 in the presence of 2.5 mmol/L [1,3-13C]glycerol
 -1,2,3-tris(methylsuccinate) or glycerol-1,2,3-tris(methyl[2,3-
 13C]succinate). The identification and quantification of
 13C-enriched metabolites by a recently developed method for the
 deconvolution of NMR (NMR) spectra with multiplet structures and
 constraints documented a virtually complete recovery of [1,3-13C
]glycerol-1,2,3-tris(methylsuccinate) in 13C-
 labeled glycerol, lactic acid, and glucose. In
 hepatocytes exposed to [1,3-13C]glycerol
 -1,2,3-tris(methylsuccinate), glucose was sym. labeled, with the
 vast majority of hexose mols. being enriched with 13C on both C1
 and C3 and/or C6 and C4. The resp. abundance of glucose
 isotopomers labeled either on both C3 and C4 or on only
 1 of these 2 C atoms indicated that the triose phosphates generated from
 [1,3-13C]glycerol represented 44% ± 1% of the total
 amount of triose phosphates incorporated into the hexose. In hepatocytes
 exposed to glycerol-1,2,3-tris(methyl[2,3-13C
]succinate), the recovery of [2,3-13C]succinate, [2,3-
 13C]fumarate, and either double- or single-labeled

malate, lactate, alanine, and glucose accounted for about half the initial ^{13C} content of the ester. The majority of the glucose mols. were now labeled in both C1 and C2 or C6 and C5, with a preferential labeling of C6-C5 relative to C1-C2, the paired C6/C1 and C5/C2 ratios averaging 1.33 ± 0.04 . These findings show that glycerol-1,2,3-tris(methylsuccinate) is efficiently and extensively metabolized in hepatocytes. They reinforce the concept that the asymmetry of glucose ^{13C}-labeling by triose phosphates generated from Krebs cycle intermediates is modulated by the availability of glycerol-derived triose phosphates. Lastly, the present study indicates that the latter triose esters, under the present exptl. conditions which do not aim at duplicating the physiol. *in vivo* situation, are largely directly channelled in the gluconeogenic pathway, with only a limited intrahepatic contribution of the "indirect" pathway involving their back-and-forth interconversion to and from pyruvate.

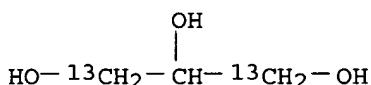
IT 102088-01-7, 1,2,3-Propanetriol-1,3-¹³C2

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis and metabolism of [1,3-¹³C]glycerol-1,2,3-tris(methylsuccinate) and glycerol-1,2,3-tris(methyl[2,3-¹³C]succinate) in rat hepatocytes)

RN 102088-01-7 HCAPLUS

CN 1,2,3-Propanetriol-1,3-¹³C2 (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:801037 HCAPLUS

DOCUMENT NUMBER: 128:101651

TITLE: Efficient syntheses of multiply ^{2H}- and ^{13C}-labeled acrylic acid, glyceric acid, glycidic acid and glycerol

AUTHOR(S): Pitlik, Janos; Townsend, Craig A.

CORPORATE SOURCE: Department of Chemistry, The Johns Hopkins University, Baltimore, MD, 21218, USA

SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1997), 39(12), 999-1009

CODEN: JLCRD4; ISSN: 0362-4803

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of multiply ^{2H}- and ^{13C}-labeled C-3 carbohydrates was carried out from com. available [1,2-¹³C2]bromoacetic acid. The syntheses are illustrated for [1,2-¹³C2]acrylate, [2,3,3-^{2H}3,1,2-¹³C2]acrylate, [1,2-¹³C2]glycerate, [2,3,3-^{2H}3,1,2-¹³C2]glycerate, [1,2-¹³C2]glycidate and [1,1-^{2H}2,1,2-¹³C2]glycerol.

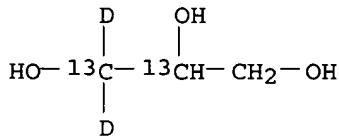
IT 201302-70-7P, 1,2,3-Propane-1,1-d2-triol-1,2-¹³C2

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of deuterated and carbon-labeled acrylic acid, glyceric acid, glycidic acid and glycerol)

RN 201302-70-7 HCAPLUS

CN 1,2,3-Propane-1,1-d2-triol-1,2-¹³C2 (9CI) (CA INDEX NAME)



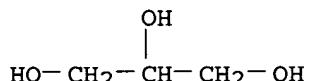
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 6 OF 20 HCPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1995:784576 HCPLUS
 DOCUMENT NUMBER: 123:222151
 TITLE: Limitations of the mass isotopomer distribution analysis of glucose to study gluconeogenesis. Substrate cycling between glycerol and triose phosphates in liver
 Previs, Stephen F.; Fernandez, Charles A.; Yang, Dawei; Soloviev, Maxim V.; David, France; Brunengraber, Henri
 AUTHOR(S): Dep. Nutr. Biomed. Eng., Case Western Reserve Univ., Cleveland, OH, 44106, USA
 CORPORATE SOURCE: Journal of Biological Chemistry (1995), 270(34), 19806-15
 SOURCE: CODEN: JBCHA3; ISSN: 0021-9258
 PUBLISHER: American Society for Biochemistry and Molecular Biology
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Mass isotopomer distribution anal. allows studying the synthesis of polymeric biomols. from 15N, 13C-, or 2H-labeled monomeric units in the presence of unlabeled polymer. The mass isotopomer distribution of the polymer allows calcn. of (1) the enrichment of the monomer and (2) the dilution of the newly synthesized polymer by unlabeled polymer. The authors tested the conditions of validity of mass isotopomer distribution anal. of glucose labeled from [U-13C3]lactate, [U-13C3]glycerol, and [2-13C]glycerol to calculate the fraction of glucose production derived from gluconeogenesis. Expts. were conducted in perfused rat livers, live rats, and live monkeys. In all cases, [13C]glycerol yielded labeling patterns of glucose that are incompatible with glucose being formed from a single pool of triose phosphates of constant enrichment. The authors show evidence that variations in the enrichment of triose phosphates result from (1) the large fractional decrease in physiol. glycerol concentration in a single pass through the liver and (2) the release of unlabeled glycerol by the liver, presumably via lipase activity. This zonation of glycerol metabolism in liver results in the calcn. of artificially low contributions of gluconeogenesis to glucose production when the latter is labeled from [13C]glycerol. In contrast, [U-13C3]lactate appears to be a suitable tracer for mass isotopomer distribution anal. of gluconeogenesis in vivo, but not in the perfused liver. In other perfusion expts. with [2H5]glycerol, the authors showed that the rat liver releases glycerol mols. containing one to four 2H atoms. This indicates the operation of a substrate cycle between extracellular glycerol and liver triose phosphates, where 2H is lost in the reversible reactions catalyzed by α -glycerophosphate dehydrogenase, triose-phosphate isomerase, and glycolytic enzymes. This substrate cycle presumably

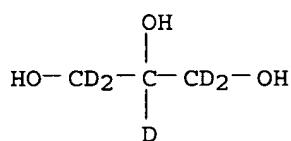
involves α -glycerophosphate hydrolysis.

IT 51767-73-8, biological studies 62502-71-0,
 1,2,3-Propane-1,1,2,3,3-d5-triol 82425-96-5,
 1,2,3-Propanetriol-2-13C
 RL: BPR (Biological process); BSU (Biological study, unclassified); BUU
 (Biological use, unclassified); BIOL (Biological study); PROC (Process);
 USES (Uses)
 (mass isotopomer anal. of glucose in gluconeogenesis and
 substrate cycling between glycerol and triose phosphates in
 liver)

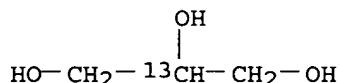
RN 51767-73-8 HCAPLUS
 CN 1,2,3-Propanetriol, labeled with carbon-13 (9CI) (CA INDEX NAME)



RN 62502-71-0 HCAPLUS
 CN 1,2,3-Propane-1,1,2,3,3-d5-triol (9CI) (CA INDEX NAME)



RN 82425-96-5 HCAPLUS
 CN 1,2,3-Propanetriol-2-13C (9CI) (CA INDEX NAME)



L25 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1995:609174 HCAPLUS
 DOCUMENT NUMBER: 123:51542
 TITLE: Quantification of compartmented metabolic fluxes in
 maize root tips using isotope distribution
 from 13C- or 14C-labeled glucose
 AUTHOR(S): Dieuaide-Noubhani, Martine; Raffard Gerard; Canioni,
 Paul; Pradet, Alain; Raymond, Philippe
 CORPORATE SOURCE: Station de Physiologie Vegetale, Institut National de
 la Recherche Agronomique, Villenave d'Ornon, 33883,
 Fr.
 SOURCE: Journal of Biological Chemistry (1995),
 270(22), 13147-59
 CODEN: JBCHA3; ISSN: 0021-9258
 PUBLISHER: American Society for Biochemistry and Molecular
 Biology
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Metabolic pathways of the intermediate metabolism of maize root tips were
 identified and quantified after labeling to isotopic

and metabolic steady state using glucose labeled on carbon-1, -2, or -6 with ^{14}C or ^{13}C . The specific radioactivity of amino acids and the ^{13}C -specific enrichment of specific carbons of free glucose, sucrose, alanine and glutamate were measured and used to calculate metabolic fluxes. The non-triose pathways, including synthesis of polysaccharides, accumulation of free hexoses, and to a lesser extent starch synthesis, were found to consume 75% of the glucose entering the root tips. The cycle of synthesis and hydrolysis of sucrose was found to consume about 70% of the ATP produced by respiration. The comparison of the specific radioactivities of amino acids and phospholipid glycerol phosphate after labeling with [$1-^{14}\text{C}$] or [$6-^{14}\text{C}$]glucose revealed the operation of the pentose phosphate pathway. The transfer of label from [$2-^{14}\text{C}$]glucose to carbon-1 of starch glucosyl units confirmed the operation of this pathway and indicated that it is located in plastids. It was found to consume 32% of the hexose phosphates entering the triose pathways. The remaining 68% were consumed by glycolysis. The determination of the specific enrichment of carbohydrate carbons -1 and -6 after labeling with [$1-^{13}\text{C}$]glucose indicated that both the conversion of triose phosphates back to hexose phosphates and the transaldolase exchange contributed to this randomization. Of the triose phosphates produced by glycolysis and the pentose phosphate pathway, about 60% were recycled to hexose phosphates, and 28% were directed to the tricarboxylic acid cycle. Of this 28%, two-thirds were directed through the pyruvate kinase branch and one-third through the phosphoenolpyruvate branch. The latter essentially has an anaplerotic function since little malate was converted to pyruvate (malic enzyme reaction).

IT 3573-62-4, D-Glucose-6- ^{14}C 3646-71-7, D-Glucose-2- ^{14}C
4005-41-8, D-Glucose-1- ^{14}C 40762-22-9, D-Glucose-1-

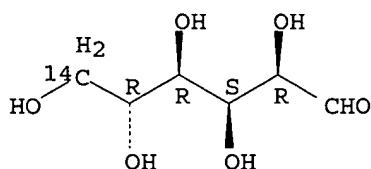
^{13}C

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses)
(quantification of compartmented metabolic fluxes in maize root tips using isotope distribution from ^{13}C - or ^{14}C -labeled glucose)

RN 3573-62-4 HCPLUS

CN D-Glucose-6- ^{14}C (7CI, 8CI, 9CI) (CA INDEX NAME)

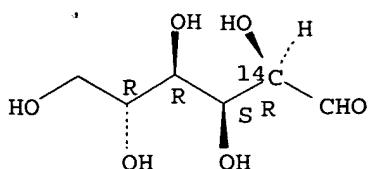
Absolute stereochemistry.



RN 3646-71-7 HCPLUS

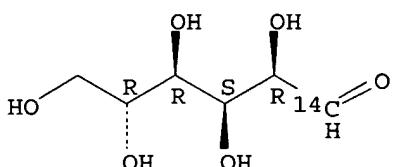
CN D-Glucose-2- ^{14}C (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



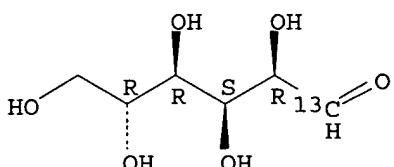
RN 4005-41-8 HCAPLUS
 CN D-Glucose-1-14C (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

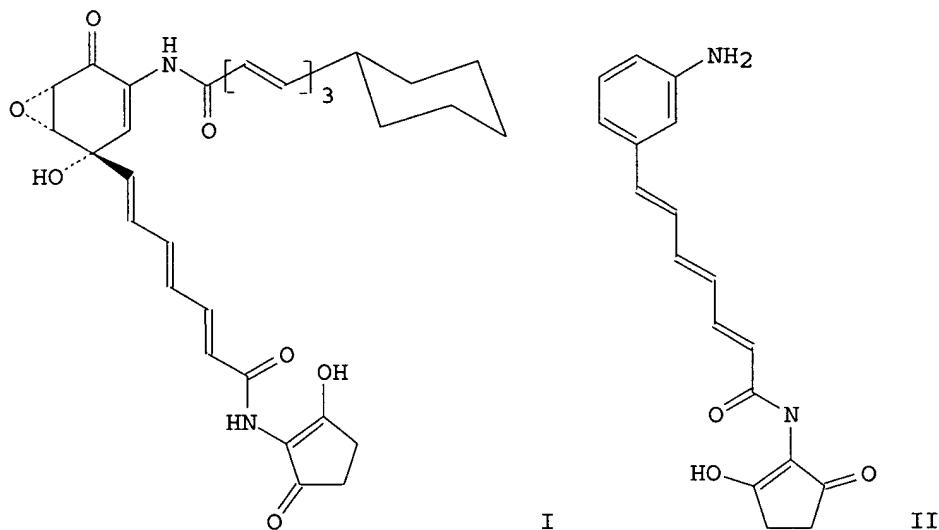


RN 40762-22-9 HCAPLUS
 CN D-Glucose-1-13C (9CI) (CA INDEX NAME)

Absolute stereochemistry.

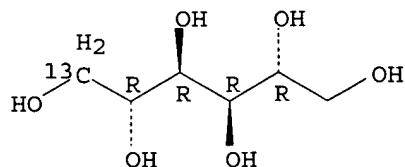


L25 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1994:239815 HCAPLUS
 DOCUMENT NUMBER: 120:239815
 TITLE: Some aspects of the stereochemistry and
biosynthesis of asukamycin
 AUTHOR(S): Cho, Hyeongjin; Sattler, Isabel; Beale, John M.;
 Zeeck, Axel; Floss, Heinz G.
 CORPORATE SOURCE: Dep. Chem., Univ. Washington, Seattle, WA, 98195, USA
 SOURCE: Journal of Organic Chemistry (1993), 58(27),
 7925-8
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



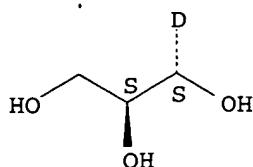
- AB High field NMR studies have established the configuration of asukamycin (I) as (4S,5R,6S), with all double bonds in the two triene chains in E configuration. Biosynthetic expts. revealed that (S)-[1-13C] glycerol labeled C(1), not C(3) of the C(7)N unit of I; the hydrogen at C(3) of I is not derived from any of the methylene hydrogens of glycerol. Feeding of m-aminobenzoic acid in high concentration to *Streptomyces nodosus* ssp. *asukaensis* resulted in the formation of a new metabolite, named asuka-mABA II.
- IT 132202-29-0, D-Mannitol-1-13C
RL: BIOL (Biological study)
(intermediate, stereochem. and biosynthesis of asukamycin)
- RN 132202-29-0 HCPLUS
CN D-Mannitol-1-13C (9CI) (CA INDEX NAME)

Absolute stereochemistry.



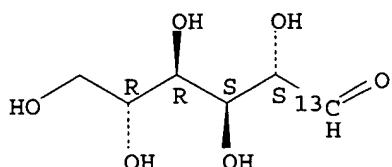
- IT 125257-42-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, stereochem. and biosynthesis of asukamycin)
- RN 125257-42-3 HCPLUS
CN 1,2,3-Propane-1-d-triol, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



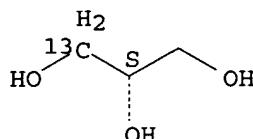
IT 70849-31-9, D-Mannose-1-13C 154278-20-3
 RL: BIOL (Biological study)
 (reactant, stereochem. and biosynthesis of asukamycin)
 RN 70849-31-9 HCPLUS
 CN D-Mannose-1-13C (9CI) (CA INDEX NAME)

Absolute stereochemistry.

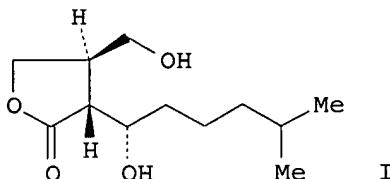


RN 154278-20-3 HCPLUS
 CN 1,2,3-Propanetriol-1-13C, (S)- (9CI) (CA INDEX NAME)

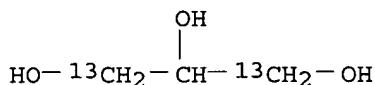
Absolute stereochemistry.



L25 ANSWER 9 OF 20 HCPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1992:55283 HCPLUS
 DOCUMENT NUMBER: 116:55283
 TITLE: Biosynthesis of virginiae butanolide A, a butyrolactone autoregulator from Streptomyces
 Sakuda, Shohei; Higashi, Ayako; Tanaka, Sumiko;
 Nihira, Takuya; Yamada, Yasuhiro
 AUTHOR(S):
 CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, 565, Japan
 SOURCE: Journal of the American Chemical Society (1992
), 114(2), 663-8
 DOCUMENT TYPE: CODEN: JACSAT; ISSN: 0002-7863
 LANGUAGE: English
 GI



- AB Virginiae butanolide A (I) is one of the virginiamycin-inducing factors from *Streptomyces virginiae* and has a unique 2,3-disubstituted butanolide skeleton which is common to other signal mols. in *Streptomyces*. The biosynthesis of I in *Streptomyces antibioticus*, a high producer of I, was studied by expts. with labeled precursors. ^{13C} and 2H NMR results as well as CI-MS analyses of dibenzoate samples indicated that the probable biosynthetic pathway to I involved coupling between a β -keto acid derivative and a C3 unit from glycerol, such as dihydroxyacetone or a derivative
- IT 102088-01-7P, 1,2,3-Propanetriol-1,3-¹³C2
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- RN 102088-01-7 HCPLUS
- CN 1,2,3-Propanetriol-1,3-¹³C2 (9CI) (CA INDEX NAME)



- L25 ANSWER 10 OF 20 HCPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:549955 HCPLUS
DOCUMENT NUMBER: 111:149955
TITLE: Rapid methods for the high yield synthesis of carbon-13 enriched intermediates of the pentose-phosphate pathway
AUTHOR(S): Arora, Krishan K.; Collins, J. Grant; MacLeod, John K.; Williams, John F.
CORPORATE SOURCE: Dep. Biochem., Aust. Natl. Univ., Canberra, Australia
SOURCE: Biological Chemistry Hoppe-Seyler (1988), 369(7), 549-57
CODEN: BCHSEI; ISSN: 0177-3593
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:149955
- AB Methods for the synthesis of carbon-13 enriched substrates, intermediates and products of the pentose-phosphate pathway, viz. ribose, arabinose, xylulose and ribulose 5-phosphates, sedoheptulose mono- and bisphosphates, octulose (both the ido- and altro-epimers) mono- and bisphosphates, are described. The procedure of the classical Kiliani synthesis was adopted for the preparation of the 2 starting compds., [1-¹³C]ribose and [1-¹³C]arabinose 5-phosphates. Using these initial reactants and enzymic methods involving the group-transferring enzymes, transketolase, aldolase and transaldolase, a variety of specifically ¹³C-labeled 5-, 6-, 7- and 8-C sugar phosphates were synthesized in high yield and purity. The isolation and authenticity of each of the ¹³C-labeled sugars

were established by column, paper and thin layer chromatog. methods and specific enzymic assays. The purity and positional isotopic anal. of these sugar-P's were confirmed by ^{13}C -NMR spectroscopy. These specifically ^{13}C -enriched compds. are required for enzymic, mechanistic and quant. investigations of pentose-pathway reactions in animal, plant and tumor tissues in vitro and in vivo.

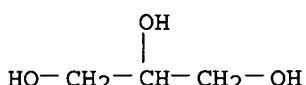
IT 51767-73-8, biological studies

RL: ANST (Analytical study)

(in preparation of carbon-13 labeled pentose phosphate pathway intermediate)

RN 51767-73-8 HCAPLUS

CN 1,2,3-Propanetriol, labeled with carbon-13 (9CI) (CA INDEX NAME)



IT 65861-56-5P

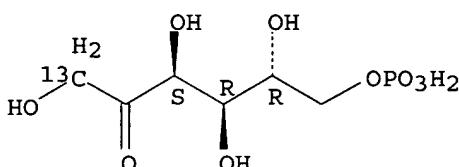
RL: PREP (Preparation)

(preparation of, as intermediate of pentose phosphate pathway)

RN 65861-56-5 HCAPLUS

CN D-Fructose-1-13C, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 84446-92-4P 84446-93-5P

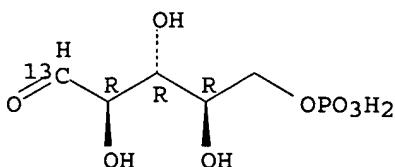
RL: PREP (Preparation)

(preparation of, as intermediate of pentose phosphate pathway, aldolase mass transfer catalysis in relation to)

RN 84446-92-4 HCAPLUS

CN D-Ribose-1-13C, 5-(dihydrogen phosphate). (9CI) (CA INDEX NAME)

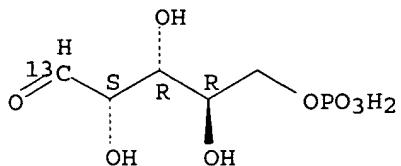
Absolute stereochemistry.



RN 84446-93-5 HCAPLUS

CN D-Arabinose-1-13C, 5-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 120388-20-7P

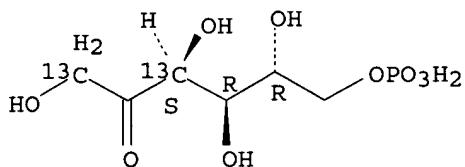
RL: PREP (Preparation)

(preparation of, as intermediate pentose phosphate pathway)

RN 120388-20-7 HCPLUS

CN D-Fructose-1,3-13C2, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 89927-01-5P 89927-04-8P 120388-06-9P

120388-07-0P 120388-08-1P 120388-09-2P

120388-12-7P 120388-13-8P 120388-21-8P

120388-23-0P 120388-24-1P, D-Glucose-5-13C

120413-17-4P 120413-19-6P 120413-20-9P

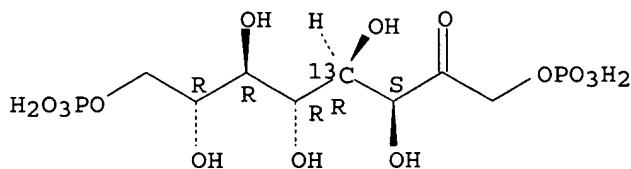
RL: PREP (Preparation)

(preparation of, as pentose phosphate pathway intermediate)

RN 89927-01-5 HCPLUS

CN D-glycero-D-alto-2-Octulose-4-13C, 1,8-bis(dihydrogen phosphate) (9CI)
(CA INDEX NAME)

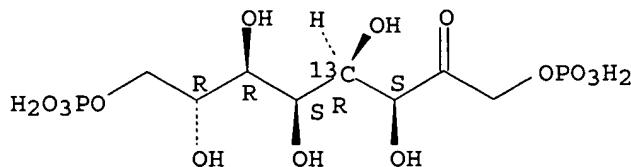
Absolute stereochemistry.



RN 89927-04-8 HCPLUS

CN D-glycero-D-ido-2-Octulose-4-13C, 1,8-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

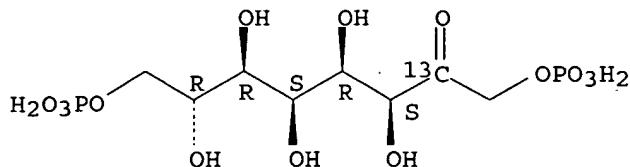
Absolute stereochemistry.



RN 120388-06-9 HCAPLUS

CN D-glycero-D-ido-2-Octulose-2-13C, 1,8-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

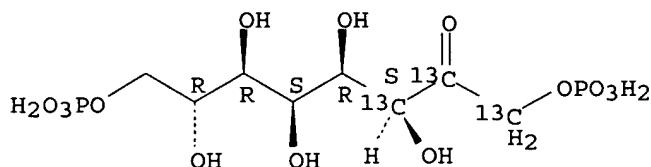
Absolute stereochemistry.



RN 120388-07-0 HCAPLUS

CN D-glycero-D-ido-2-Octulose-1,2,3-13C3, 1,8-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

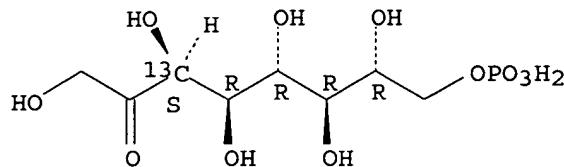
Absolute stereochemistry.



RN 120388-08-1 HCAPLUS

CN D-glycero-D-altrio-2-Octulose-3-13C, 8-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

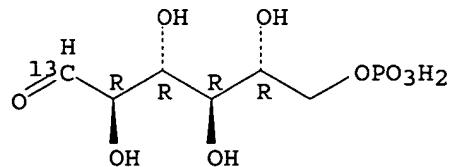
Absolute stereochemistry.



RN 120388-09-2 HCAPLUS

CN D-Allose-1-13C, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

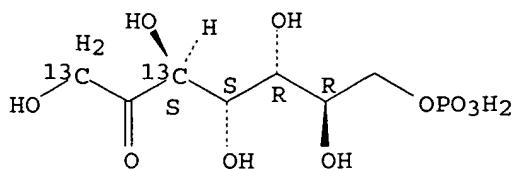
Absolute stereochemistry.



RN 120388-12-7 HCAPLUS

CN D-manno-2-Heptulose-1,3-13C2, 7-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

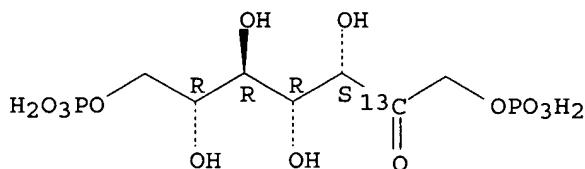
Absolute stereochemistry.



RN 120388-13-8 HCPLUS

CN D-altro-2-Heptulose-2-13C, 1,7-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

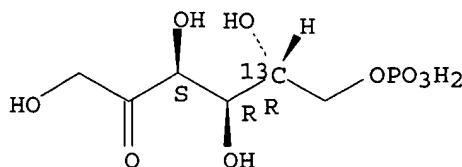
Absolute stereochemistry.



RN 120388-21-8 HCPLUS

CN D-Fructose-5-13C, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

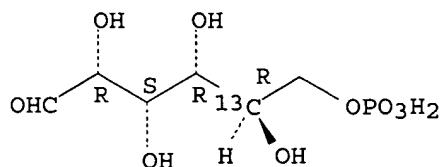
Absolute stereochemistry.



RN 120388-23-0 HCPLUS

CN D-Glucose-5-13C, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

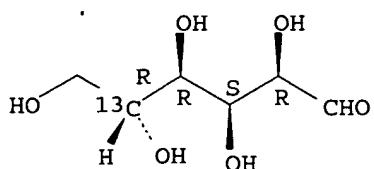
Absolute stereochemistry.



RN 120388-24-1 HCPLUS

CN D-Glucose-5-13C (9CI) (CA INDEX NAME)

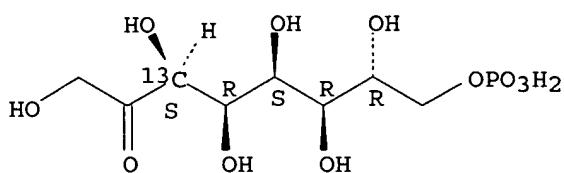
Absolute stereochemistry.



RN 120413-17-4 HCAPLUS

CN D-glycero-D-ido-2-Octulose-3-13C, 8-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

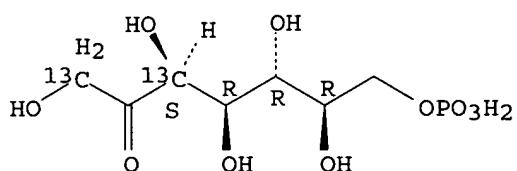
Absolute stereochemistry.



RN 120413-19-6 HCAPLUS

CN D-altro-2-Heptulose-1,3-13C2, 7-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

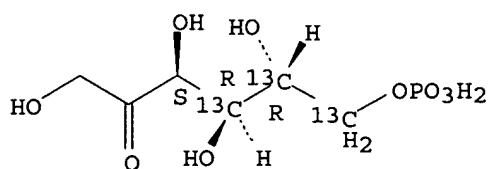
Absolute stereochemistry.



RN 120413-20-9 HCAPLUS

CN D-Fructose-4,5,6-13C3, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

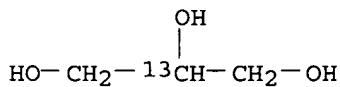


IT 82425-96-5, 1,2,3-Propanetriol-2-13C

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with glycerol phosphate dehydrogenase)

RN 82425-96-5 HCAPLUS

CN 1,2,3-Propanetriol-2-13C (9CI) (CA INDEX NAME)



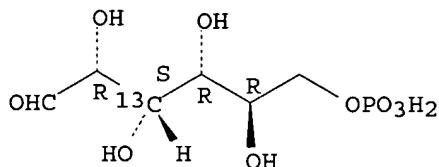
IT 120388-10-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (transketolase catalyzed reactions of, in carbon-13 labeled
 pentose phosphate pathway intermediates)

RN 120388-10-5 HCPLUS

CN D-Glucose-3-13C, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L25 ANSWER 11 OF 20 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:570733 HCPLUS

DOCUMENT NUMBER: 109:170733

TITLE: The synthesis of carbon-13-enriched monosaccharides derived from glucose and mannose

AUTHOR(S): Walker, Thomas E.; Unkefer, Clifford J.; Ehler, Deborah S.

CORPORATE SOURCE: Los Alamos Natl. Lab., Univ. California, Los Alamos, NM, 87545, USA

SOURCE: Journal of Carbohydrate Chemistry (1988), 7(1), 115-32

CODEN: JCACDM; ISSN: 0732-8303

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:170733

AB A modified Kiliani-Fischer reaction is used to prepare multigram quantities of [1-13C]-enriched glucose and mannose which are converted chemically or enzymically into other labeled monosaccharides. The simplest conversion is the synthesis of labeled fructose from labeled glucose using com. available immobilized glucose isomerase. The equilibrium for this reaction provides a 1:1 mixture of glucose and fructose which can be separated by chromatog. The equilibrium can

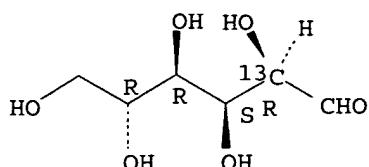
be shifted toward fructose by treating the reaction with germanate ion. [1-13C]Mannose can be converted into more useful sugars using a modification of the Lobry de Bruyn-Alberda van Ekenstein transformation. In this reaction, D-[1-13C]mannose is treated with an aqueous solution of dilute alkali and phenylboronate to form a mixture of labeled fructose, mannose and glucose. Fructose can be converted to a mixture of Me fructofuranosides by using trifluoroacetic acid in methanol. [2-13C]Dihydroxyacetone can be prepared from Me D-[2-13C]fructose by treatment with periodate followed by reduction with borohydride and acid hydrolysis.

IT 70849-17-1, D-Glucose-2-13C

RL: RCT (Reactant); RACT (Reactant or reagent)
 (enzymic isomerization of)

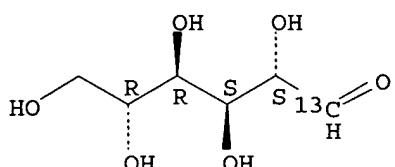
RN 70849-17-1 HCAPLUS
 CN D-Glucose-2-13C (9CI) (CA INDEX NAME)

Absolute stereochemistry.



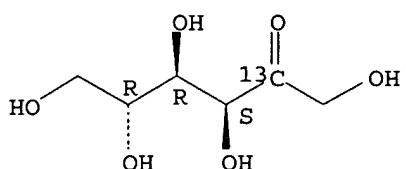
IT 70849-31-9, D-Mannose-1-13C
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (isomerization of, in presence of phenylboronic acid)
 RN 70849-31-9 HCAPLUS
 CN D-Mannose-1-13C (9CI) (CA INDEX NAME)

Absolute stereochemistry.



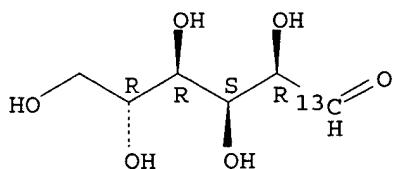
IT 117013-19-1P, D-Fructose-2-13C
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and glycosidation of, with methanol)
 RN 117013-19-1 HCAPLUS
 CN D-Fructose-2-13C (9CI) (CA INDEX NAME)

Absolute stereochemistry.



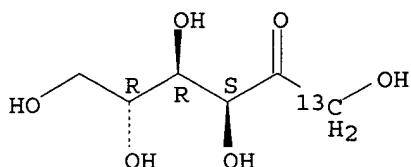
IT 40762-22-9P, D-Glucose-1-13C 108311-21-3P,
 D-Fructose-1-13C
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 40762-22-9 HCAPLUS
 CN D-Glucose-1-13C (9CI) (CA INDEX NAME)

Absolute stereochemistry.



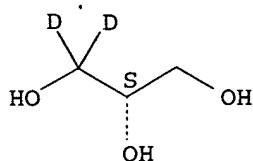
RN 108311-21-3 HCAPLUS
 CN D-Fructose-1-13C (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L25 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1987:530636 HCAPLUS
 DOCUMENT NUMBER: 107:130636
 TITLE: The regiochemistry and stereochemistry of the biosynthesis of vitamin B6 from triose units
 Hill, Robert E.; Iwanow, Agnieszka; Sayer, Brian G.; Wysocka, Waleria; Spenser, Ian D.
 AUTHOR(S): Dep. Chem., McMaster Univ., Hamilton, ON, L8S 4M1, Can.
 CORPORATE SOURCE:
 SOURCE: Journal of Biological Chemistry (1987), 262(16), 7463-71
 CODEN: JBCHA3; ISSN: 0021-9258
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB **13C** and **2H-NMR** spectroscopy were used to probe the biosynthesis of vitamin B6 in *Escherichia coli*. The **13C** NMR spectrum of a sample of pyridoxol derived biosynthetically from D-[1,2,3,4,5,6-13C6]glucose shows that the bonds, C(2)-C(3) and C(4)-C(5), of the pyridine nucleus are the only 2 C-C bonds of pyridoxol which are generated de novo in the course of its biosynthesis from glucose. It follows that the pyridoxol skeleton is generated from 2 intact triose units and a triose-derived 2-carbon unit, all of which are supplied by glucose. From the **2H** NMR spectra of samples of pyridoxol derived from (R)-[1,1-2H2]glycerol and (S)-[1,1-2H2]glycerol, resp., it can be deduced that the re-hydroxymethyl group of glycerol enters C-2', C-4', and C-5' of the pyridoxol skeleton. It follows that each of the 3 fragments is derived from glycerol in stereospecific fashion. These results answer questions concerning the regiochem. and the stereochem. of pyridoxol biosynthesis.
 IT 110270-11-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, for study of vitamin B6 biosynthesis)
 RN 110270-11-6 HCAPLUS.
 CN 1,2,3-Propane-1,1-d2-triol, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



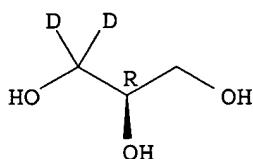
IT 62532-65-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in study of biosynthesis of vitamin B6)

RN 62532-65-4 HCAPLUS

CN 1,2,3-*Propane-1,1-d*₂-triol, (2*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



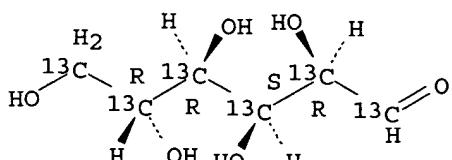
IT 110187-42-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in study of vitamin B6 biosynthesis)

RN 110187-42-3 HCAPLUS

CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



I-25 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2006 ACS ON STN

ACCESSION NUMBER: 1987:455447 HCAPLUS

ACCESSION NUMBER: 1987.4554
DOCUMENT NUMBER: 107:55447

DOCUMENT NUMBER: 107-33447 TITLE: Studies on the biosynthesis of tabtoxin

TITLE: Studies on the biosynthesis of tabtoxin (wildfire toxin). Origin of the carbonyl C-atom of the β -lactam moiety from the C1-pool

Mueller, Barbara; Haedener, Alfons; Tamm, Christoph

CORPORATE SOURCE: Inst. Org. Chem., Univ. Basel, Basel, CH-4056

SOURCE: Inst. Org. Chem., Univ. Basel, Basel, CH-4056
Helvetica Chimica Acta (1987), 70(2), 412-22

HELVETICA CHIMICA ACTA (1987),
CODEN: HCACAV; ISSN: 0018-018X

DOCUMENT TYPE: Journal

DOCUMENT TYPE: Journal
LANGUAGE: English

AB Reisolation of *Pseudomonas tabaci* strain NCPPB 2730 from its host, the tobacco plant, led to an activation of the bacteria to produce the β -lactam dipeptide tabtoxin (Wildfire toxin, I). Incorporation of several ¹⁴C-labeled amino acids as well as L-[methyl-¹³C]methionine, L-[1,2-¹³C₂] - and L-[3,4-¹³C₂]aspartate, rac-[1,2-¹³C₂] glycerol, and [1,2-¹³C₂]acetate into isotabtoxin demonstrated that

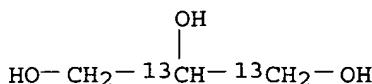
the building blocks of I are L-threonine, L-aspartate, the Me group of L-methionine and a C2-unit derived from the C3-pool. The Me group of L-methionine provides the carbonyl C-atom of the β -lactam moiety. These findings represent a novel pathway in β -lactam biosynthesis. Mechanistic aspects with respect to the β -lactam ring formation are discussed. A biradical is proposed as an intermediate during the cyclization of a N-formyl- α -amino ketone.

IT 109376-40-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and isotabtoxin incorporation of, in Pseudomonas tabaci)

RN 109376-40-1 HCPLUS

CN 1,2,3-Propanetriol-1,2-13C2 (9CI) (CA INDEX NAME)



SENT REQUEST.

L25 ANSWER 14 OF 20 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:523831 HCPLUS

DOCUMENT NUMBER: 103:123831

TITLE: Total synthesis of (1-13C)-glycerol

AUTHOR(S): Barber, Jill

CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, OX1 3QU, UK

SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals
(1985), 22(3), 229-34

CODEN: JLCRD4; ISSN: 0362-4803

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:123831

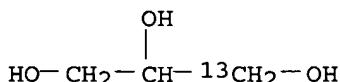
AB PhCH₂OCH₂CHO, prepared from HOCH₂CH(OEt)₂ by benzylation with PhCH₂Cl followed by hydrolysis with H₂O-H₂SO₄, was treated with K¹³CN in H₂O in the presence of NH₄Cl to give PhCH₂OCH₂CH(OH)¹³CN, which on refluxing with MeOH in the presence of H₂SO₄ gave PhCH₂OCH₂CH(OH)¹³CO₂Me, which on reduction with LiAlH₄ followed by hydrogenolysis gave the title compound HOCH₂CH(OH)¹³CH₂OH.

IT 98292-00-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 98292-00-3 HCPLUS

CN 1,2,3-Propanetriol-1-13C (9CI) (CA INDEX NAME)



L25 ANSWER 15 OF 20 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:520653 HCPLUS

DOCUMENT NUMBER: 99:120653

TITLE: Synthesis of sugars by aldolase-catalyzed condensation reactions

AUTHOR(S): Wong, Chi Huey; Whitesides, George M.

CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02138, USA

SOURCE: Journal of Organic Chemistry (1983), 48(19),
3199-205
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:120653

AB Dihydroxyacetone phosphate [57-04-5] was prepared in 200-mmol scale from dihydroxyacetone [96-26-4] by 2 procedures: (1) reaction with POCl₃ and (2) glycerol kinase [9030-66-4]-catalyzed phosphorylation using ATP [56-65-5] with in situ regeneration of ATP by phosphoenolpyruvate [138-08-9] or acetyl phosphate [590-54-5]. Dihydroxyacetone phosphate was converted to fructose 6-phosphate [643-13-0] in 80% yield by exposure to a mixture of coimmobilized triosephosphate isomerase [9023-78-3] and aldolase [9024-52-6] followed by acid hydrolysis of the condensation product fructose 1,6-bis(phosphate) [488-69-7]. Fructose 6-phosphate was subsequently converted by chemical and enzymic schemes into fructose [30237-26-4], glucose 6-phosphate [56-73-5], and glucose [50-99-7]. Practical procedures are described for the preparation of D- [591-57-1] and L-glyceraldehyde 3-phosphate [20283-52-7] and for several hexoses labeled with ¹³C in the C-2 and C-2,5 positions.

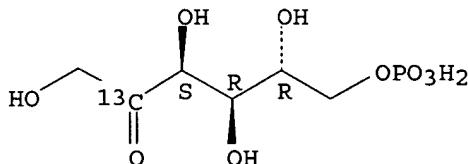
IT 86595-23-5P

RL: PREP (Preparation)
(preparation of)

RN 86595-23-5 HCAPLUS

CN D-Fructose-2-13C, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 70849-17-1P 84270-11-1P 84270-12-2P

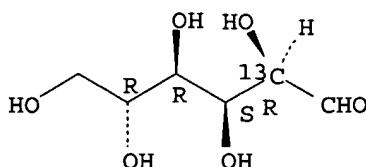
86595-19-9P 86595-24-6P 86595-25-7P

RL: PREP (Preparation)
(preparation of, enzymic)

RN 70849-17-1 HCAPLUS

CN D-Glucose-2-13C (9CI) (CA INDEX NAME)

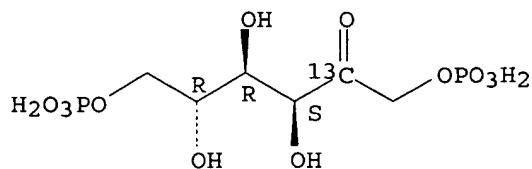
Absolute stereochemistry.



RN 84270-11-1 HCAPLUS

CN D-Fructose-2-13C, 1,6-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

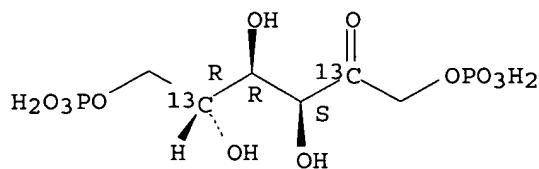
Absolute stereochemistry.



RN 84270-12-2 HCPLUS

CN D-Fructose-2,5-13C2, 1,6-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

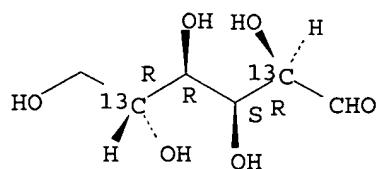
Absolute stereochemistry.



RN 86595-19-9 HCPLUS

CN D-Glucose-2,5-13C2 (9CI) (CA INDEX NAME)

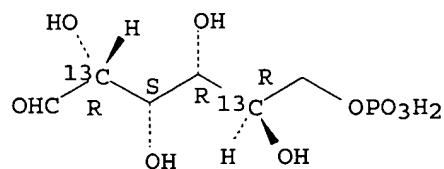
Absolute stereochemistry.



RN 86595-24-6 HCPLUS

CN D-Glucose-2,5-13C2, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

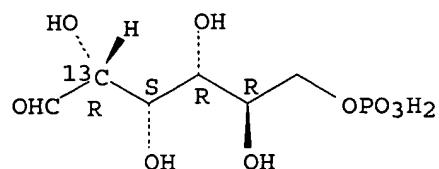
Absolute stereochemistry.



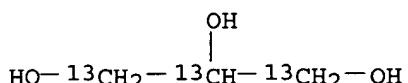
RN 86595-25-7 HCPLUS

CN D-Glucose-2-13C, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

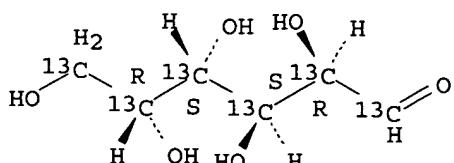


L25 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1980:586689 HCAPLUS
 DOCUMENT NUMBER: 93:186689
 TITLE: Photosynthetic preparation of galactose-13C6 and glycerol-13C3 using a marine red alga
 AUTHOR(S): Kollman, V. H.; London, R. E.; Hanners, J. L.; Gregg, C. T.; Whaley, T. W.
 CORPORATE SOURCE: Los Alamos Sci. Lab., Univ. California, Los Alamos, NM, 87545, USA
 SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1979), 16(6), 833-42
 CODEN: JLCRD4; ISSN: 0362-4803
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Gigartina corymbifera Formed 2-hydroxy-1-(hydroxymethyl)ethyl α -D-galactopyranoside-U- 13C (I) during photosynthesis in 13CO₂. I was isolated from an alc. extract by an acetylation procedure and subsequently hydrolyzed to D-galactose-13C6 and glycerol-13C3. The average enrichment of the isolated products was 55 mol % 13C whereas the actual enrichment of newly synthesized material determined by 13C NMR, was 80 mol % 13C after a photosynthetic period of 48 h during which 90 mol % 13CO₂ was administered. The administered 13C was recovered in 30% yield in the products and the average 13C/12C ratio for each compound was 54 mol %.
 IT 63346-81-6P 74134-89-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (photosynthetic preparation of, using Gigartina corymbifera)
 RN 63346-81-6 HCAPLUS
 CN 1,2,3-Propanetriol-1,2,3-13C3 (9CI) (CA INDEX NAME)



RN 74134-89-7 HCAPLUS
 CN D-Galactose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

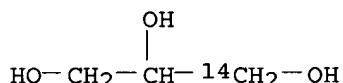


L25 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1980:426312 HCAPLUS
 DOCUMENT NUMBER: 93:26312
 TITLE: Studies on the biosynthesis of clavulanic acid. II. Chemical degradations of carbon-14-labeled clavulanic acid
 AUTHOR(S): Stirling, Irene; Elson, S. W.

CORPORATE SOURCE: Res. Div., Beecham Pharm., Betchworth/Surrey, RH3 7AJ,
UK
SOURCE: Journal of Antibiotics (1979), 32(11),
1125-9
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two chemical degradns. of clavulanic acid are described which are useful for locating the label in ¹⁴C-clavulanate. In the first, the β-hydroxyethylidene side chain of p-bromobenzyl clavulanate (I) was removed by ozonolysis to give p-bromobenzyl (2R,5R)-3,7-dioxo-4-oxa-1-azabicyclo[3.2.0]heptane-2-carboxylate. The second involved the reaction of I with dibenzylamine in MeOH to give the 3 β-lactam carbons as Me trans-3-(dibenzylamino)acrylate. These techniques were used to degrade clavulanic acid derived from fermns. fed with 2-¹⁴C-acetate or universally **¹⁴C-labeled glycerol**. The amount of label retained in the degradation products was in agreement with the distribution of ¹³C in clavulanic acid derived from 2-¹³C-acetate, or 1,3-¹³C₂-glycerol, as observed by ¹³C NMR.

IT 56-80-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(biosynthesis of clavulanic acid from, carbon-14 distribution in)
RN 56-80-4 HCAPLUS
CN 1,2,3-Propanetriol-1-¹⁴C (9CI) (CA INDEX NAME)



L25 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:59835 HCAPLUS
DOCUMENT NUMBER: 88:59835
TITLE: Biosynthetic and biophysical information from carbon-13/carbon-13 multiplets by carbon-13 nuclear magnetic resonance
AUTHOR(S): London, R. E.; Kollman, V. H.; Matwiyoff, N. A.; Mueller, D. D.
CORPORATE SOURCE: Los Alamos Sci. Lab., Univ. California, Los Alamos, NM, USA
SOURCE: Proc. Int. Conf. Stable Isot., 2nd (1976), Meeting Date 1975, 470-84. Editor(s): Klein, E. Roseland; Klein, Peter D. NTIS: Springfield, Va.
CODEN: 37EVA5
DOCUMENT TYPE: Conference
LANGUAGE: English
AB ¹³C-enriched mols. exhibit multiplets due to ¹³C-¹³C scalar coupling, the relative intensities of which are related quant. to the percentage enrichment of the C atoms. Thus, ¹³C enrichment during the course of a biosynthetic experiment can be monitored by an anal. of the ¹³C-¹³C multiplet intensities. In addition, multiplet peaks provide a way of measuring a correlation in the ¹³C labeling of scalar-coupled C atoms. Biophys. measurements are based on the ¹³C-¹³C dipolar coupling that can provide a significant contribution to the relaxation of nonprotonated C atoms. This technique is useful for studying internal rotation that will affect the ratio of the ¹³C-¹H to the

¹³C-¹³C dipolar coupling. Examples of each type of application are presented. The photosynthetic fixation of ¹³CO₂ into 2-hydroxy-1-(hydroxymethyl)ethyl α-D-galactopyranoside (galactosyl glycerol) by species of the marine red alga, *Gigartina*, was studied by these methods. Algal samples were then taken at various times after the initial exposure to ¹³CO₂, and the galactosyl glycerol was extracted NMR and mass spectrometric measurements indicated that the galactosyl glycerol consists of a pool of unlabeled material and a pool of newly synthesized material, the labeling of which increases as time progresses. In addition, spin lattice relaxation and nuclear Overhauser enhancement (NOE) measurements of ¹³C-¹³C multiplets of 6-phosphogluconate were made. Measurements made in D₂O on the carboxyl C resonances were compared with calculated T₁ and NOE values for singlet and doublet lines. Anisotropic rotation of the mol. was indicated.

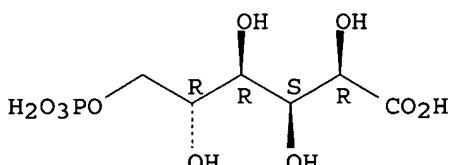
IT 65445-43-4

RL: ANST (Analytical study)
(carbon-13 NMR multiplet anal. of)

RN 65445-43-4 HCPLUS

CN D-Gluconic acid, 6-(dihydrogen phosphate), labeled with carbon-13 (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L25 ANSWER 19 OF 20 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1976:541034 HCPLUS

DOCUMENT NUMBER: 85:141034

TITLE: Incorporation of D-[3-³H, U-¹⁴C]-glucose into glycerolipid via acyl dihydroxyacetone phosphate in untransformed and viral-transformed BHK-21-^{c13} fibroblasts

AUTHOR(S): Pollock, Robert J.; Hajra, Amiya; Agranoff, Bernard W.

CORPORATE SOURCE: Ment. Health Res. Inst., Univ. Michigan, Ann Arbor, MI, USA

SOURCE: Journal of Biological Chemistry (1976), 251(17), 5149-54
CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Untransformed BHK-21-^{c13} fibroblasts as well as 4 polyoma-transformed strains were incubated with D-glucose-U-¹⁴C, ³H. This substrate generates intracellular labeled glycerol and also NADPH-4-³H. The latter selectively transfers H to C-2 of glycerol in glycerolipid via the acyl dihydroxyacetone phosphate pathway. After incubation, the distribution of radioactivity and the ratios of ³H/¹⁴C at the 3 positions of recovered glycerol were determined in sn-glycerol 3-phosphate, saponifiable glycerolipids, alkyl ether glycerolipids, and plasmalogens. In each of the cell types examined, ³H in the sn-1 position of glycerol in the recovered ether-containing glycerolipids was negligible, yet this position contained most of the recovered ³H in

sn-glycerol 3-phosphate and saponifiable glycerolipids
 . The 3H/14C ratio in position 2 of **glycerol**, measured at various incubation times, was 5- to 200-fold greater in the saponifiable **glycerolipids** than in free **sn-glycerol 3-phosphate**. The ratio in position 2 of ether-containing **glycerolipids** was the same or greater than that in the saponifiable **glycerolipids** in all of the cell types employed. A similar pattern in the 3H/14C ratio was observed when BHK-21-c13 cells were incubated with D-glucose-U-14C, 1-3H. These data demonstrate significant participation of the acyl dihydroxyacetone phosphate pathway in **glycerolipid synthesis** in BHK cells.

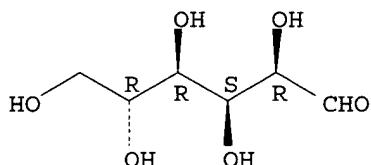
IT 60771-22-4

RL: PROC (Process)
 (glycerolipid incorporation of, in transformed fibroblast)

RN 60771-22-4 HCPLUS

CN D-Glucose-t, labeled with carbon-14 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L25 ANSWER 20 OF 20 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1974:34890 HCPLUS

DOCUMENT NUMBER: 80:34890

TITLE: Large-scale photosynthetic production of carbon-13 labeled sugars

AUTHOR(S): Kollman, V. H.; Gregg, C. T.; Hanners, J. L.; Whaley, T. W.; Ott, D. G.

CORPORATE SOURCE: Los Alamos Sci. Lab., NM, USA

SOURCE: Report (1973), LA-UR-73-690, 25 pp. Avail.:

Dep. NTIS

From: Nucl. Sci. Abstr. 1973, 28(6), 12712

DOCUMENT TYPE: Report

LANGUAGE: English

AB A large-scale preparation of uniformly ¹³C-labeled sugars using young, mature leaves from tobacco, Swiss chard, canna plants, and thalli of marine red algae is described. The tobacco system produces primarily starch, with lesser amts. of free glucose, fructose, and sucrose. Swiss chard and cannas produce the 3 simple carbohydrates. Galactose and **glycerol** are obtained from the marine red algae Gigartina.

IT 19030-38-7P, preparation 51767-72-7P, preparation

51767-73-8P, preparation

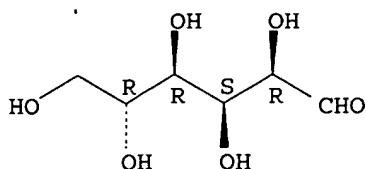
RL: PREP (Preparation)

(photosynthetic)

RN 19030-38-7 HCPLUS

CN D-Glucose, labeled with carbon-13 (8CI, 9CI) (CA INDEX NAME)

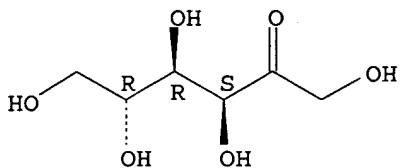
Absolute stereochemistry.



RN 51767-72-7 HCAPLUS

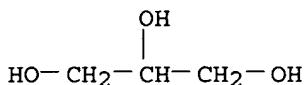
CN D-Fructose, labeled with carbon-13 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 51767-73-8 HCAPLUS

CN 1,2,3-Propanetriol, labeled with carbon-13 (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 16:03:26 ON 08 AUG 2006)

FILE 'HCAPLUS' ENTERED AT 16:34:23 ON 08 AUG 2006

E MARTINEZ RODOLFO/AU

L1 29 S E3-5

E UNKERER CLIFFORD J/AU

L2 83 S E1-4

E ALVAREZ MARC A/AU

L3 9 S E2-3

L4 6 S L1 AND L2 AND L3

L5 5 S L4 AND ?ISOTOP?

L6 1 S L5 AND ?GLYCEROL?

SELECT RN L6 1

FILE 'REGISTRY' ENTERED AT 16:35:50 ON 08 AUG 2006

L7 60 S E1-60

FILE 'HCAPLUS' ENTERED AT 16:35:59 ON 08 AUG 2006

L8 1 S L6 AND L7

L9 ANALYZE L8 1 CT : 2 TERMS

FILE 'HCAPLUS' ENTERED AT 16:42:27 ON 08 AUG 2006

FILE 'REGISTRY' ENTERED AT 16:42:30 ON 08 AUG 2006

L10 STR

L11 50 S L10
L12 72312 S L10 FUL
L13 0 S L12 AND 2039
L14 0 S L12 AND SCR 2039
L15 SCREEN 2039
L16 SCREEN 2045
L17 50 S L10 AND L15
L18 50 S L10 AND (L15 OR L16)
L19 2049 S L10 AND (L15 OR L16) FUL

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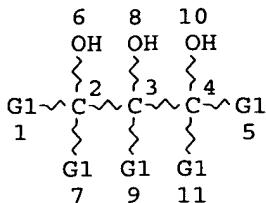
L20 3350 S L19
L21 1971 S L20 AND (?ISOTOP? OR ?LABEL?)
L22 157 S L21 AND ?GLYCEROL?
L23 62 S L22 AND ?SYNTHESIS?
L24 58 S L23 AND (PRD<20030730 OR PD<20030730)
L25 20 S L24 AND (C12 OR 12C OR C13 OR 13C)

FILE 'USPATFULL' ENTERED AT 16:54:40 ON 08 AUG 2006

L26 17 S L25

FILE 'HCAPLUS' ENTERED AT 16:55:19 ON 08 AUG 2006

=> d que stat 126
L10 . STR



VAR G1=H/D
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L15 SCR 2039
L16 SCR 2045
L19 2049 SEA FILE=REGISTRY SSS FUL L10 AND (L15 OR L16)
L20 3350 SEA FILE=HCAPLUS ABB=ON L19
L21 1971 SEA FILE=HCAPLUS ABB=ON L20 AND (?ISOTOP? OR ?LABEL?)
L22 157 SEA FILE=HCAPLUS ABB=ON L21 AND ?GLYCEROL?
L23 62 SEA FILE=HCAPLUS ABB=ON L22 AND ?SYNTHESIS?
L24 58 SEA FILE=HCAPLUS ABB=ON L23 AND (PRD<20030730 OR PD<20030730)
L26 17 SEA FILE=USPATFULL ABB=ON L24 AND (C12 OR 12C OR C13 OR 13C)

=> d ibib abs hitstr 126 1-17

L26 ANSWER 1 OF 17 USPATFULL on STN
ACCESSION NUMBER: 2006:86484 USPATFULL
TITLE: Mass defect labeling for the determination of oligomer sequences
INVENTOR(S): Schneider, Luke V., Half Moon Bay, CA, UNITED STATES
Hall, Michael P., San Carlos, CA, UNITED STATES
Petesch, Robert, Newark, CA, UNITED STATES
PATENT ASSIGNEE(S): Taget Discovery, Inc., Palo Alto, CA, UNITED STATES
(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2006073485	A1	20060406
APPLICATION INFO.:	US 2004-913020	A1	20040806 (10)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 2001-35349, filed on 19 Oct 2001, GRANTED, Pat. No. US 6962818		

	NUMBER	DATE	
PRIORITY INFORMATION:	US 2000-242165P	20001019 (60)	<--
	US 2000-242398P	20001019 (60)	<--
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	TOWNSEND AND TOWNSEND AND CREW, LLP, TWO EMBARCADERO CENTER, EIGHTH FLOOR, SAN FRANCISCO, CA, 94111-3834, US		
NUMBER OF CLAIMS:	19		
EXEMPLARY CLAIM:	1-50		

NUMBER OF DRAWINGS: 32 Drawing Page(s)

LINE COUNT: 3323

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Mass tagging methods are provided that lead to mass spectrometer detection sensitivities and molecular discriminations that are improved over other methods. In particular the methods are useful for discriminating tagged molecules and fragments of molecules from chemical noise in the mass spectrum. These mass tagging methods are useful for oligomer sequencing, determining the relative abundances of molecules from different samples, and identifying individual molecules or chemical processing steps in combinatorial chemical libraries. The methods provided are useful for the simultaneous analysis of multiple molecules and reaction mixtures by mass spectrometric methods.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

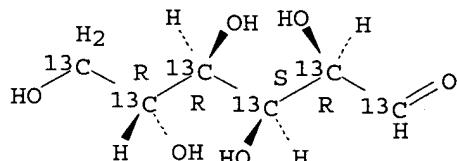
IT 110187-42-3, [13C]6-Glucose

(detecting metabolites of, in Escherichia coli; polypeptide fingerprinting methods and metabolic profiling and apparatus and bioinformatics database)

RN 110187-42-3 USPATFULL

CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 2 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2005:177266 USPATFULL

TITLE: Methods for conducting metabolic analyses

INVENTOR(S): Schneider, Luke V., Half Moon Bay, CA, UNITED STATES

PATENT ASSIGNEE(S): Target Discovery, Inc., Palo Alto, CA, UNITED STATES
(U.S. corporation)

NUMBER KIND DATE

PATENT INFORMATION: US 2005153346 A1 20050714

APPLICATION INFO.: US 2004-18871 A1 20041220 (11)

RELATED APPLN. INFO.: Continuation of Ser. No. US 2003-687909, filed on 17 Oct 2003, GRANTED, Pat. No. US 6849396 Continuation of Ser. No. US 2000-553424, filed on 19 Apr 2000, GRANTED, Pat. No. US 6764817

NUMBER DATE

PRIORITY INFORMATION: US 1999-130238P 19990420 (60) <--

DOCUMENT TYPE: Utility

FILE SEGMENT: APPLICATION

LEGAL REPRESENTATIVE: TOWNSEND AND TOWNSEND AND CREW, LLP, TWO EMBARCADERO CENTER, EIGHTH FLOOR, SAN FRANCISCO, CA, 94111-3834, US

NUMBER OF CLAIMS: 22

EXEMPLARY CLAIM: 1

NUMBER OF DRAWINGS: 28 Drawing Page(s)

LINE COUNT: 2855

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB . The present invention provides methods and apparatus for purifying metabolites of interest and conducting metabolic analyses. The methods generally involve determining metabolic flux values for a plurality of target analytes by monitoring the relative *isotope* abundance of a stable *isotope* in a substrate labeled with the stable *isotope* and/or one or more target metabolites formed through metabolism of the labeled substrate. Certain methods utilize multiple electrophoretic methods to separate the target analytes from other components within the sample being analyzed. The methods can be used in a variety of applications including screens to identify metabolites that are correlated with certain diseases and diagnostic screens for identifying individuals having, or susceptible to, a disease.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

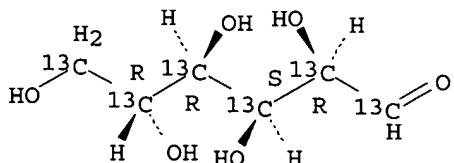
IT 110187-42-3, [13C]6-Glucose

(detecting metabolites of, in Escherichia coli; polypeptide fingerprinting methods and metabolic profiling and apparatus and bioinformatics database)

RN 110187-42-3 USPATFULL

CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 3 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2005:104994 USPATFULL
 TITLE: Polypeptide fingerprinting methods
 INVENTOR(S): Schneider, Luke V., Half Moon Bay, CA, UNITED STATES
 Hall, Michael P., San Carlos, CA, UNITED STATES
 Petesch, Robert, Newark, CA, UNITED STATES
 Peterson, Jeffrey N., Foster City, CA, UNITED STATES
 PATENT ASSIGNEE(S): Target Discovery, Inc., Palo Alto, CA, UNITED STATES
 (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2005089930	A1	20050428
APPLICATION INFO.:	US 2003-721047	A1	20031121 (10)
RELATED APPLN. INFO.:	Division of Ser. No. US 2000-513907, filed on 25 Feb 2000, GRANTED, Pat. No. US 6677114		

	NUMBER	DATE	
PRIORITY INFORMATION:	US 1999-130238P	19990420 (60)	<--
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	TOWNSEND AND TOWNSEND AND CREW, LLP, TWO EMBARCADERO CENTER, EIGHTH FLOOR, SAN FRANCISCO, CA, 94111-3834, US		
NUMBER OF CLAIMS:	10		
EXEMPLARY CLAIM:	1-21		

NUMBER OF DRAWINGS: 29 Drawing Page(s)

LINE COUNT: 4732

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention provides methods, compositions, apparatus, and a computer data retrieval system for conducting proteomics.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

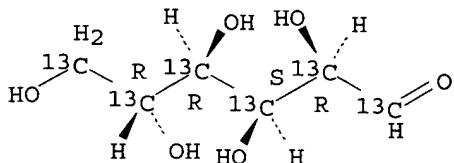
IT 110187-42-3, [13C]6-Glucose

(detecting metabolites of, in Escherichia coli; polypeptide fingerprinting methods and metabolic profiling and apparatus and bioinformatics database)

RN 110187-42-3 USPATFULL

CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 4 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2004:313853 USPATFULL

TITLE: Simultaneous dual *isotope* imaging of cardiac perfusion and cardiac inflammation

INVENTOR(S): Carpenter, Alan P., JR., Carlisle, MA, UNITED STATES

PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company (U.S. corporation)

NUMBER	KIND	DATE
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PATENT INFORMATION: US 2004247523 A1 20041209

APPLICATION INFO.: US 2004-865457 A1 20040610 (10)

RELATED APPLN. INFO.: Division of Ser. No. US 2001-2359, filed on 2 Nov 2001,
GRANTED, Pat. No. US 6770259

NUMBER	DATE
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PRIORITY INFORMATION: US 2000-245554P 20001103 (60) <--
DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: BRISTOL - MYERS SQUIBB COMPANY, PO BOX 4000, PRINCETON,
NJ, 08543-4000

NUMBER OF CLAIMS: 13

EXEMPLARY CLAIM: 1

LINE COUNT: 8710

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides novel diagnostic compositions comprising a **radiolabeled** LTB4 binding agent and a **radiolabeled** perfusion imaging agent, diagnostic kits comprising such compositions, and methods of concurrent imaging in a mammal comprising administering a **radiolabeled** LTB4 binding agent and a **radiolabeled** perfusion imaging agent, and concurrently detecting the **radiolabeled** LTB4 binding agent bound at the LTB4 receptor and the **radiolabeled** perfusion imaging agent.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

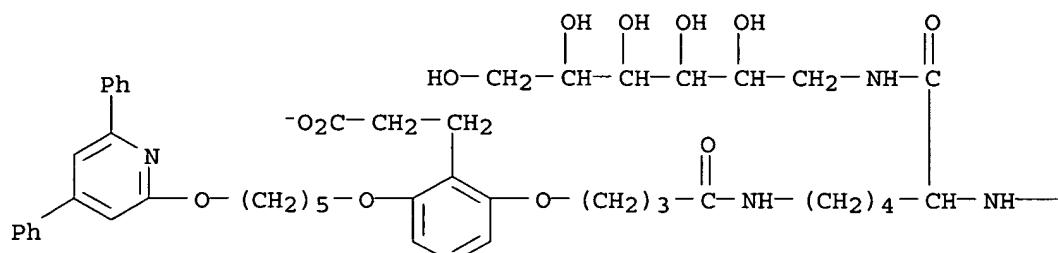
IT 206264-10-0P 206264-13-3P 206264-48-4P
 206264-51-9P 206264-53-1P 206264-67-7P

(preparation of 99m Tc complexes with leukotriene antagonist ligands for simultaneous dual isotope imaging of perfusion and inflammation)

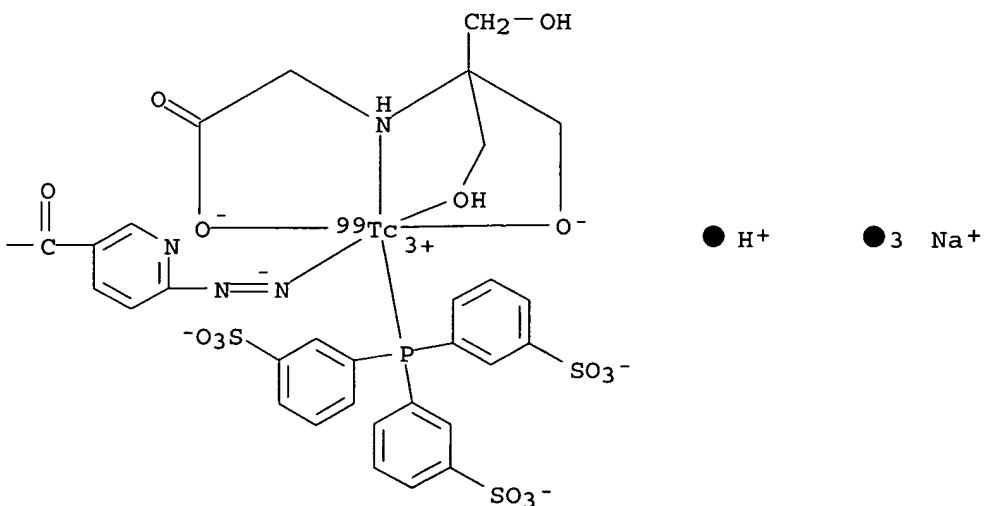
RN 206264-10-0 USPATFULL

CN Technetate (4-) - 99 Tc, [1-[[6-[[4-[2-(2-carboxyethyl)-3-[[5-[(4,6-diphenyl-2-pyridinyl)oxy]pentyl]oxy]phenoxy]-1-oxobutyl]amino]-2-[[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato(2-)][[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium hydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



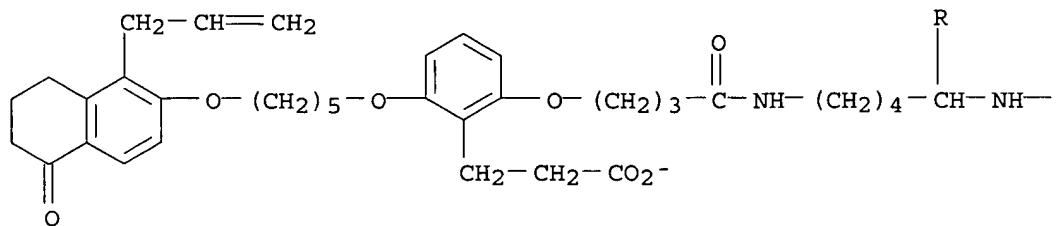
PAGE 1-B



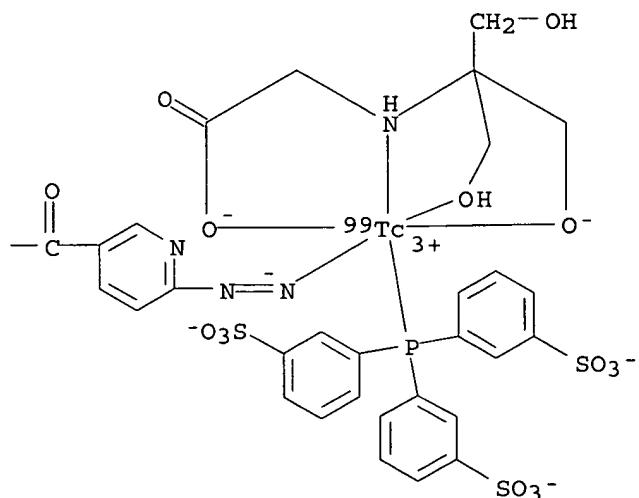
RN 206264-13-3 USPATFULL

CN Technetate (4-) - 99 Tc, [1-[[6-[[4-[2-(2-carboxyethyl)-3-[[5,6,7,8-tetrahydro-5-oxo-1-(2-propenyl)-2-naphthalenyl]oxy]pentyl]oxy]phenoxy]-1-oxobutyl]amino]-2-[[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-8-glucitolato(2-)][[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium hydrogen (9CI) (CA INDEX NAME)

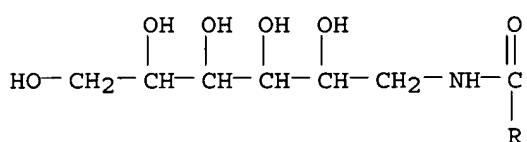
PAGE 1-A



PAGE 1-B



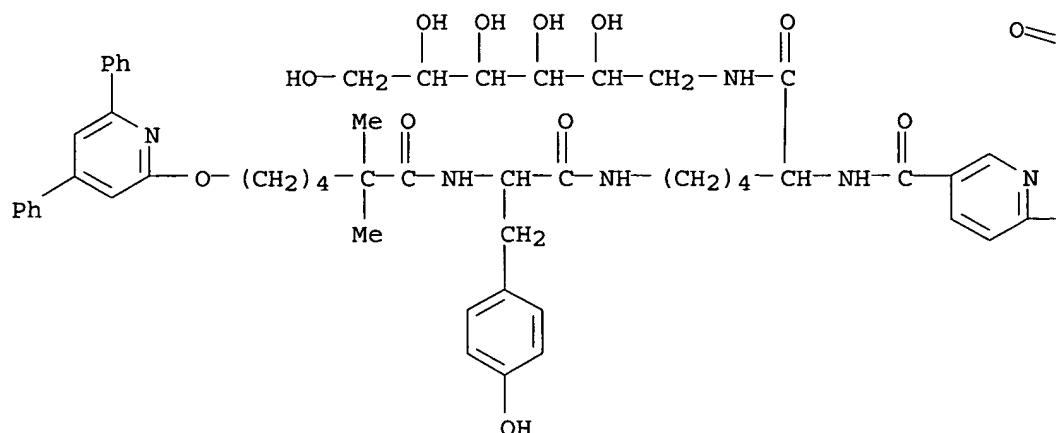
PAGE 2-A

 $\bullet \text{H}^+$ $\bullet 3 \text{ Na}^+$

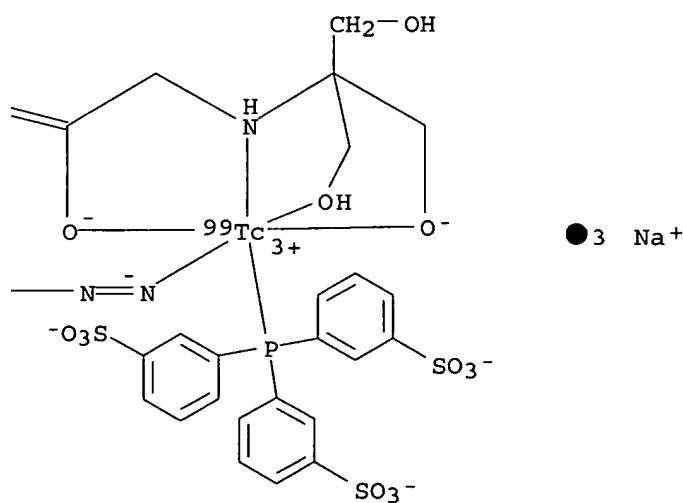
RN 206264-48-4 USPATFULL

CN Technetate(3-) -99Tc, [1-deoxy-1-[[N2-[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]-N6-[N-[6-[(4,6-diphenyl-2-pyridinyl)oxy]-2,2-dimethyl-1-oxohexyl]-L-tyrosyl]-L-lysyl]amino]-D-glucitolato] [N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinato(2-)- κ N, κ O] [[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

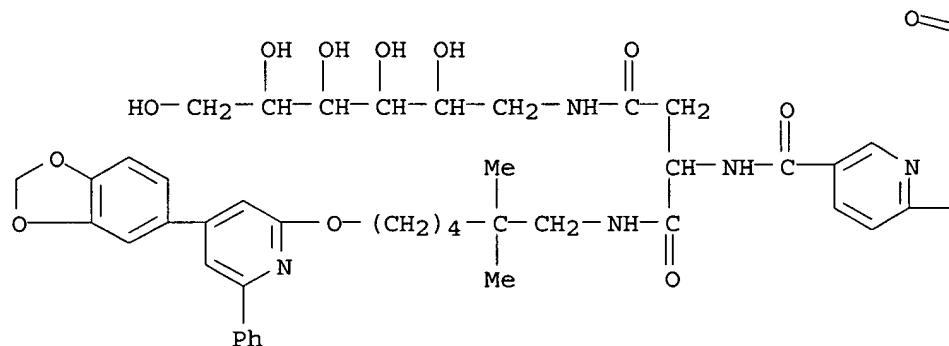


RN 206264-51-9 USPATFULL

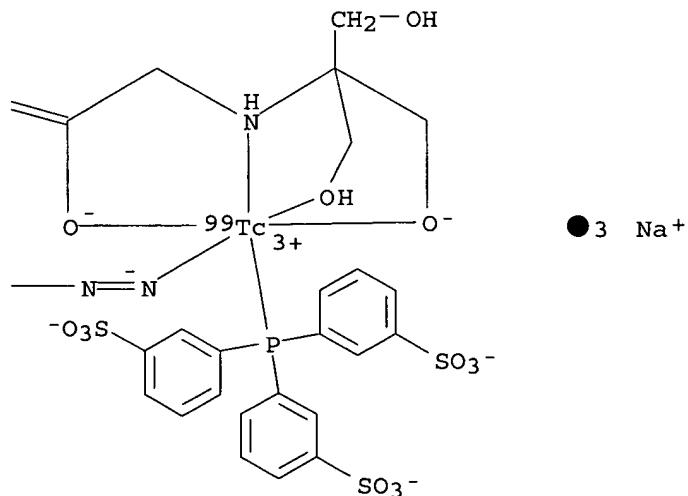
CN Technetate(3-) -99Tc, [1-[[4-[[6-[[4-(1,3-benzodioxol-5-yl)-6-phenyl-2-pyridinyl]oxy]-2,2-dimethylhexyl]amino]-3-[[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]amino]-1,4-dioxobutyl]amino]-1-deoxy-D-glucitolato] [N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinato(2-)-

$\kappa N, \kappa O$ [[3,3',3'''-(phosphinidyne- κP)tris[benzenesulfonato]](3-)]-, trisodium (9CI) (CA INDEX NAME)

PAGE 1-A



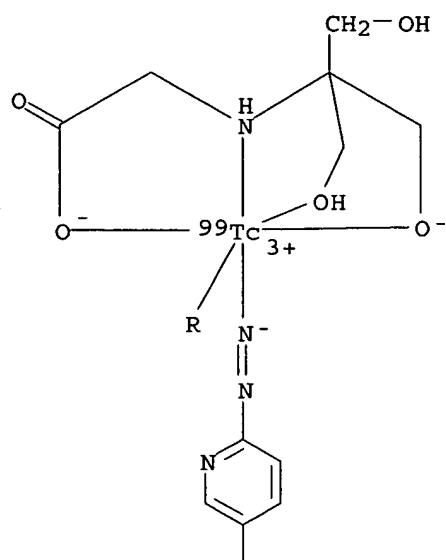
PAGE 1-B



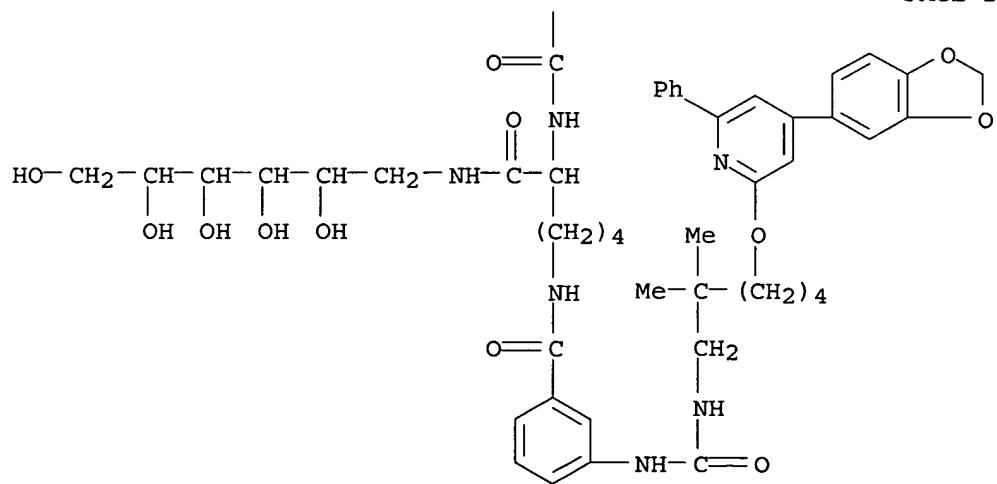
RN 206264-53-1 USPATFULL

CN Technetate(3-) - 99Tc, [1-[6-[[3-[[[6-[[4-(1,3-benzodioxol-5-yl)-6-phenyl-2-pyridinyl]oxy]-2,2-dimethylhexyl]amino]carbonyl]amino]benzoyl]amino]-2-[[[6-(diazenyl- $\kappa N2$)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato][N-[2-hydroxy-1,1-bis[(hydroxy- κO)methyl]ethyl]glycinato(2-) - $\kappa N, \kappa O$ [[3,3',3'''-(phosphinidyne- κP)tris[benzenesulfonato]](3-)]-, trisodium (9CI) (CA INDEX NAME)

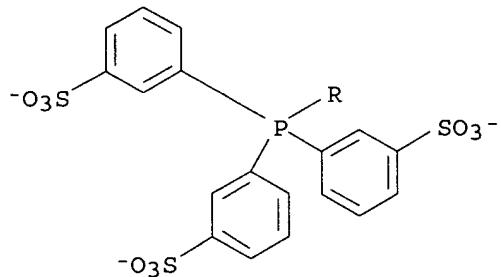
PAGE 1-A



PAGE 2-A



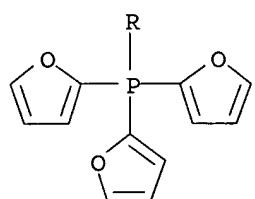
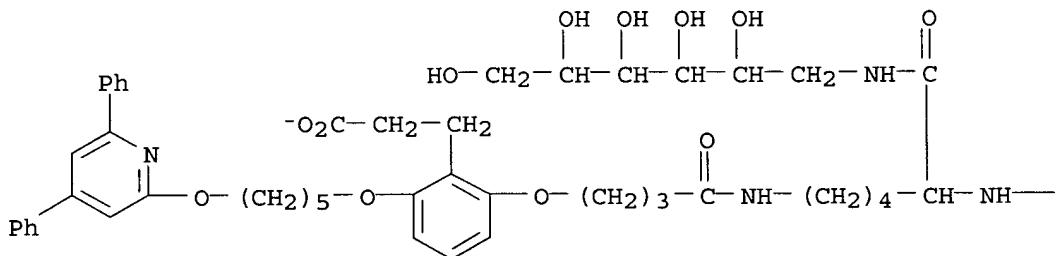
PAGE 3-A

● 3 Na⁺

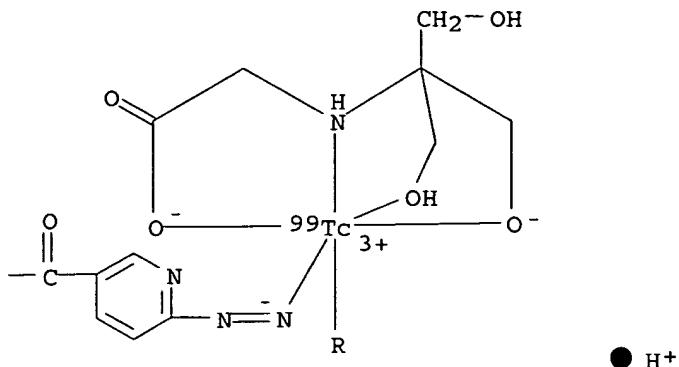
RN 206264-67-7 USPATFULL

CN Technetate(1-) - 99Tc, [1-[[6-[[4-[2-(2-carboxyethyl)-3-[[5-[(4,6-diphenyl-2-pyridinyl)oxy]pentyl]oxy]phenoxy]-1-oxobutyl]amino]-2-[[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato(2-)] [N-[2-hydroxy-1,1-bis([hydroxy- κ O)methyl]ethyl]glycinato(2-)- κ N, κ O] (tri-2-furanylphosphine- κ P)-, hydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L26 ANSWER 5 OF 17 USPATFULL on STN
 ACCESSION NUMBER: 2004:267711 USPATFULL
 TITLE: Methods for determining protein and peptide terminal sequences
 INVENTOR(S): Schneider, Luke V., Half Moon Bay, CA, UNITED STATES
 Hall, Michael P., Hayward, CA, UNITED STATES
 Petesch, Robert, Newark, CA, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004209251	A1	20041021
APPLICATION INFO.:	US 2001-33303	A1	20011019 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2000-242165P	20001019 (60)
	US 2000-242398P	20001019 (60)

DOCUMENT TYPE: Utility
 FILE SEGMENT: APPLICATION
 LEGAL REPRESENTATIVE: James C. Scheller, Jr., BLAKELY, SOKOLOFF, TAYLOR & ZAFMAN LLP, 7th Floor, 12400 Wilshire Boulevard, Los Angeles, CA, 90025

NUMBER OF CLAIMS: 114
 EXEMPLARY CLAIM: 1
 NUMBER OF DRAWINGS: 39 Drawing Page(s)
 LINE COUNT: 3924

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Methods and apparatuses for deriving the sequence of an oligomer. In one exemplary method for deriving the sequence of a polypeptide, a predetermined set of mass/charge values for amino acid sequences is stored. An abundance value from mass spectrum data for each mass/charge value in the predetermined set is determined to produce a plurality of abundance values. A first ranking, based on the plurality of abundance values, is calculated for each sequence of a set of amino acid sequences having a first number of amino acids. A second ranking, based on the plurality of abundance values, for each sequence of a set of amino acid sequences having a second number of amino acids is calculated. A cumulative ranking, based on the first ranking and the second ranking, is calculated for each sequence of a set of amino acid sequences having at least the second number of amino acids.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

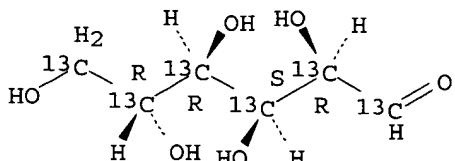
IT 110187-42-3, [13C]6-Glucose

(detecting metabolites of, in Escherichia coli; polypeptide fingerprinting methods and metabolic profiling and apparatus and bioinformatics database)

RN 110187-42-3 USPATFULL

CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 6 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2004:181011 USPATFULL

TITLE: Methods for conducting metabolic analyses

INVENTOR(S): Schneider, Luke V., Half Moon Bay, CA, United States

PATENT ASSIGNEE(S): Target Discovery, Inc., Palo Alto, CA, United States
(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6764817	B1	20040720
APPLICATION INFO.:	US 2000-553424		20000419 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-130238P	19990420 (60) <--
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Leary, Louise N.	
LEGAL REPRESENTATIVE:	Townsend and Townsend and Crew LLP	
NUMBER OF CLAIMS:	35	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	1 Drawing Figure(s); 28 Drawing Page(s)	
LINE COUNT:	2985	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides methods and apparatus for purifying metabolites of interest and conducting metabolic analyses. The methods generally involve determining metabolic flux values for a plurality of target analytes by monitoring the relative isotope abundance of a stable isotope in a substrate labeled with the stable isotope and/or one or more target metabolites formed through metabolism of the labeled substrate. Certain methods utilize multiple electrophoretic methods to separate the target analytes from other components within the sample being analyzed. The methods can be used in a variety of applications including screens to identify metabolites that are correlated with certain diseases and diagnostic screens for identifying individuals having, or susceptible to, a disease.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 110187-42-3, [13C]6-Glucose

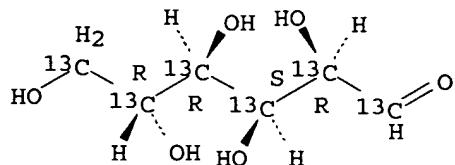
(detecting metabolites of, in Escherichia coli; polypeptide

fingerprinting methods and metabolic profiling and apparatus and
bioinformatics database)

RN 110187-42-3 USPATFULL

CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 7 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2004:150910 USPATFULL

TITLE:

Deuterated glucose or fat tolerance tests for
high-throughput measurement of the metabolism of sugars
or fatty acids in the body

INVENTOR(S): Hellerstein, Marc K., Kensington, CA, UNITED STATES

PATENT ASSIGNEE(S): The Regents of the University of California, Oakland,
CA, 94607-5200 (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004115131	A1	20040617
APPLICATION INFO.:	US 2003-701990	A1	20031104 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2002-423964P	20021104 (60) <--
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	MORRISON & FOERSTER LLP, 425 MARKET STREET, SAN FRANCISCO, CA, 94105-2482	
NUMBER OF CLAIMS:	66	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	6 Drawing Page(s)	
LINE COUNT:	1439	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Provided herein are methods for determining the metabolism of one or more sugars and/or fatty acids, and applications thereof. Such applications include determining the rate of glycogen synthesis and glycolysis, which are believed to be early markers for predicting elevated risk of diabetes and cardiovascular disease. Other applications include methods for screening drugs that effect sugar and/or fatty acid metabolism. The methods are useful for at least partially characterizing drugs for desirable or undesirable (toxic) characteristics. Drugs that are at least partially characterized using the methods of the invention can then be further developed in pre-clinical testing and clinical trials. Such drugs may be found to be useful in treating obesity, diabetes, cardiovascular disease, and other disorders of metabolism.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

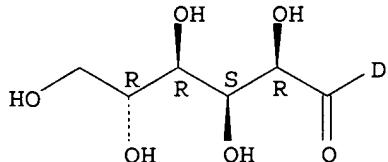
IT 10390-17-7, D-Glucose-1-C-d 18991-62-3,

D-Glucose-6,6-C-d2 66034-51-3

(deuterated glucose or fat tolerance tests for high-throughput measurement of metabolism of sugars or fatty acids in body)

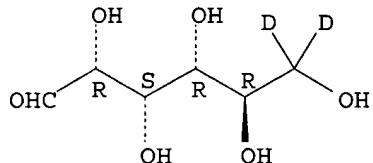
RN 10390-17-7 USPATFULL
 CN D-Glucose-1-C-d (9CI) (CA INDEX NAME)

Absolute stereochemistry.



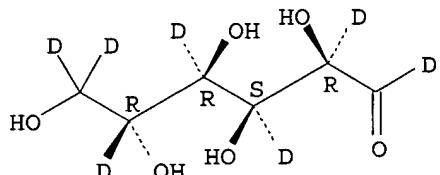
RN 18991-62-3 USPATFULL
 CN D-Glucose-6,6-C-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 66034-51-3 USPATFULL
 CN D-Glucose-1,2,3,4,5,6-C-d7 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 8 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2004:120533 USPATFULL
 TITLE: Methods for conducting metabolic analyses
 INVENTOR(S): Schneider, Luke V., Half Moon Bay, CA, UNITED STATES
 PATENT ASSIGNEE(S): Target Discovery, Inc., Palo Alto, CA (U.S.
 corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004091943	A1	20040513
	US 6849396	B2	20050201
APPLICATION INFO.:	US 2003-687909	A1	20031017 (10)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 2000-553424, filed on 19 Apr 2000, PENDING		

	NUMBER	DATE	
PRIORITY INFORMATION:	US 1999-130238P	19990420 (60)	<--
DOCUMENT TYPE:	Utility		

FILE SEGMENT: APPLICATION
 LEGAL REPRESENTATIVE: TOWNSEND AND TOWNSEND AND CREW, LLP, TWO EMBARCADERO CENTER, EIGHTH FLOOR, SAN FRANCISCO, CA, 94111-3834
 NUMBER OF CLAIMS: 38
 EXEMPLARY CLAIM: 1
 NUMBER OF DRAWINGS: 28 Drawing Page(s)
 LINE COUNT: 2997

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides methods and apparatus for purifying metabolites of interest and conducting metabolic analyses. The methods generally involve determining metabolic flux values for a plurality of target analytes by monitoring the relative isotope abundance of a stable isotope in a substrate labeled with the stable isotope and/or one or more target metabolites formed through metabolism of the labeled substrate. Certain methods utilize multiple electrophoretic methods to separate the target analytes from other components within the sample being analyzed. The methods can be used in a variety of applications including screens to identify metabolites that are correlated with certain diseases and diagnostic screens for identifying individuals having, or susceptible to, a disease.

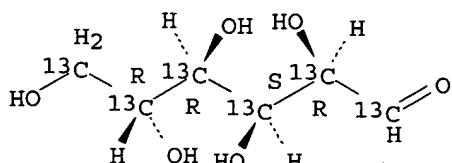
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 110187-42-3, [13C]6-Glucose
 (detecting metabolites of, in Escherichia coli; polypeptide fingerprinting methods and metabolic profiling and apparatus and bioinformatics database)

RN 110187-42-3 USPATFULL

CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 9 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2004:107594 USPATFULL
 TITLE: Biochemical methods for measuring metabolic fitness of tissues or whole organisms
 INVENTOR(S): Hellerstein, Marc K., Kensington, CA, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004081994	A1	20040429
APPLICATION INFO.:	US 2003-664513	A1	20030916 (10)

	NUMBER	DATE	
PRIORITY INFORMATION:	US 2002-411029P	20020916 (60)	<--
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	MORRISON & FOERSTER LLP, 425 MARKET STREET, SAN FRANCISCO, CA, 94105-2482		
NUMBER OF CLAIMS:	58		

EXEMPLARY CLAIM:

1

NUMBER OF DRAWINGS: 10 Drawing Page(s)

LINE COUNT: 1634

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to biochemical methods for assessing metabolic fitness and/or aerobic demands of a living system. Specifically, the rate of **synthesis** and turnover of the molecular components of mitochondrial mass are used to determine the aerobic capacity and/or aerobic demand of tissues or living organisms. The direct measurement of metabolic fitness and/or aerobic demand by this means can be used as an index of the efficacy of an exercise training program or other therapeutic intervention; as a medical risk factor for predicting the risk of cardiovascular disease, diabetes, death or other health outcome; or as an aid to pharmaceutical companies for drug discovery in the area of metabolic fitness, deconditioning, and oxidative biology.

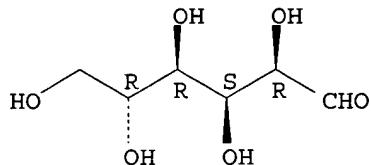
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 815-92-9, biological studies 19030-38-7, biological studies 28823-03-2, biological studies 50938-64-2, biological studies (biochem. methods for measuring metabolic fitness of tissues or whole organisms)

RN 815-92-9 USPATFULL

CN D-Glucose, labeled with carbon-14 (9CI) (CA INDEX NAME)

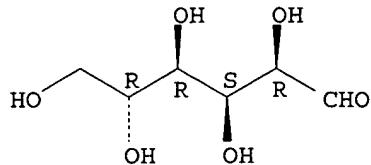
Absolute stereochemistry.



RN 19030-38-7 USPATFULL

CN D-Glucose, labeled with carbon-13 (8CI, 9CI) (CA INDEX NAME)

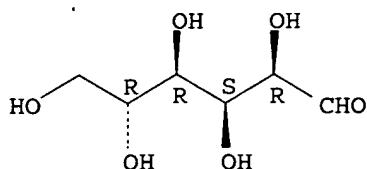
Absolute stereochemistry.



RN 28823-03-2 USPATFULL

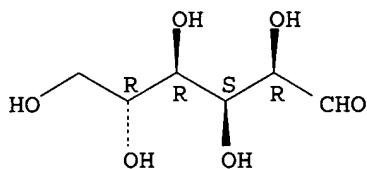
CN D-Glucose, labeled with tritium (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 50938-64-2 USPATFULL
 CN D-Glucose, labeled with deuterium (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 10 OF 17 USPATFULL on STN
 ACCESSION NUMBER: 2004:9525 USPATFULL
 TITLE: Polypeptide fingerprinting methods and bioinformatics database system
 INVENTOR(S): Schneider, Luke V., Half Moon Bay, CA, United States
 Hall, Michael P., San Carlos, CA, United States
 Petesch, Robert, Newark, CA, United States
 Peterson, Jeffrey N., Foster City, CA, United States
 PATENT ASSIGNEE(S): Target Discovery, Inc., Palo Alto, CA, United States
 (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6677114	B1	20040113
APPLICATION INFO.:	US 2000-513907		20000225 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-130238P	19990420 (60) <--
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Horlick, Kenneth R.	
ASSISTANT EXAMINER:	Kim, Young	
LEGAL REPRESENTATIVE:	Townsend and Townsend and Crew LLP	
NUMBER OF CLAIMS:	16	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	31 Drawing Figure(s); 29 Drawing Page(s)	
LINE COUNT:	4788	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention provides methods, compositions, apparatus, and a computer data retrieval system for conducting proteomics.

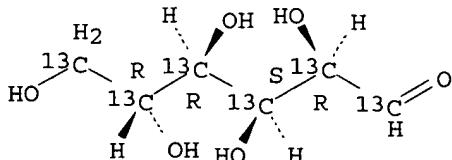
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 110187-42-3, [13C]6-Glucose

(detecting metabolites of, in *Escherichia coli*; polypeptide fingerprinting methods and metabolic profiling and apparatus and bioinformatics database)

RN 110187-42-3 USPATFULL
 CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 11 OF 17 USPATFULL on STN
 ACCESSION NUMBER: 2003:180226 USPATFULL
 TITLE: Radiopharmaceuticals for imaging infection and inflammation
 INVENTOR(S): Barrett, John Andrew, West Groton, MA, UNITED STATES
 Cheesman, Edward Hollister, Lunenburg, MA, UNITED STATES
 Harris, Thomas David, Salem, NH, UNITED STATES
 Liu, Shuang, Chelmsford, MA, UNITED STATES
 Rajopadhye, Milind, Westford, MA, UNITED STATES
 Sworin, Michael, Tyngsboro, MA, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2003124053	A1	20030703 <--
APPLICATION INFO.:	US 2002-151663	A1	20020520 (10)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1997-943659, filed on 3 Oct 1997, GRANTED, Pat. No. US 6416733		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1996-27955P	19961007 (60) <--
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	STEPHEN B. DAVIS, BRISTOL-MYERS SQUIBB COMPANY, PATENT DEPARTMENT, P O BOX 4000, PRINCETON, NJ, 08543-4000	
NUMBER OF CLAIMS:	26	
EXEMPLARY CLAIM:	1	
LINE COUNT:	9146	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides novel radiopharmaceuticals useful for the diagnosis of infection and inflammation, reagents and kits useful for preparing the radiopharmaceuticals, methods of imaging sites of infection and/or inflammation in a patient, and methods of diagnosing diseases associated with infection or inflammation in patients in need of such diagnosis. The radiopharmaceuticals bind in vivo to the leukotriene B4 (LTB4) receptor on the surface of leukocytes which accumulate at the site of infection and inflammation. The reagents provided by this invention are also useful for the treatment of diseases associated with infection and inflammation.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

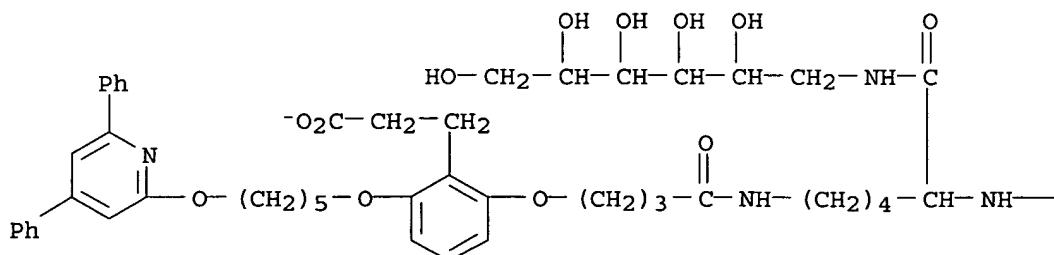
IT 206264-10-0P, Technetate(4-) -99Tc, [1-[[6-[[4-[2-(2-carboxyethyl)-3-[[5-[(4,6-diphenyl-2-pyridinyl)oxy]pentyl]oxy]phenoxy]-1-oxobutyl]amino]-2-[[[6-(diazaryl- κ N2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato(2-)][[3,3',3''-(phosphinidyne-

κ P)tris[benzenesulfonato](3-)]-, trisodium hydrogen
206264-13-3P **206264-48-4P**, Technetate(3-)-99Tc,
 [1-deoxy-1-[[N2-[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]-N6-[6-
 [(4,6-diphenyl-2-pyridinyl)oxy]-2,2-dimethyl-1-oxohexyl]-L-tyrosyl]-L-
 lysyl]amino]-D-glucitolato][N-[2-hydroxy-1,1-bis[(hydroxy-
 κ O)methyl]ethyl]glycinato(2-)- κ N, κ O][[3,3',3'''-
 (phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium
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 glucitolato][N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinat
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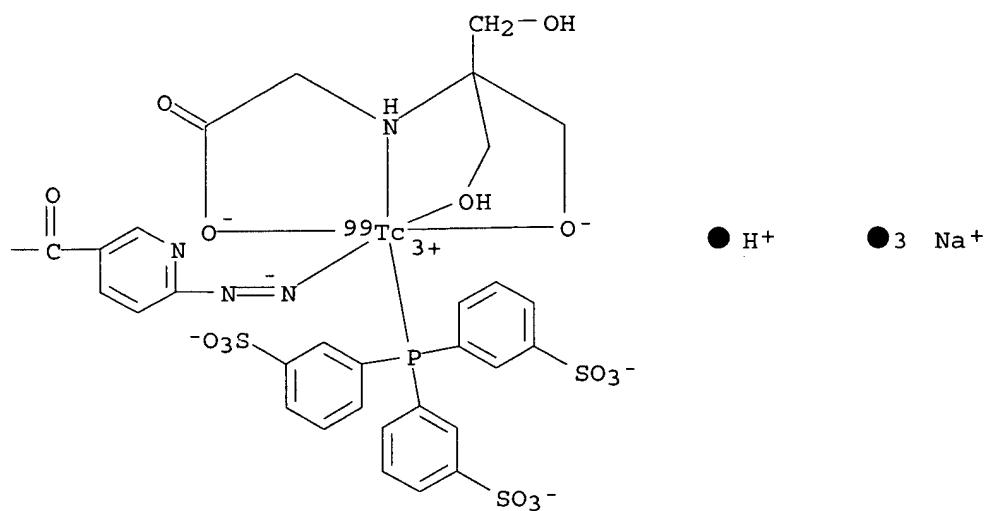
(preparation of 99mTc complexes with leukotriene antagonist ligands for
 imaging and treatment of infection and inflammation)

RN 206264-10-0 USPATFULL
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PAGE 1-A



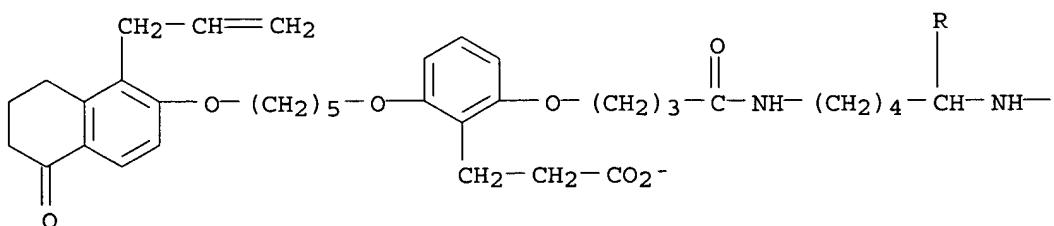
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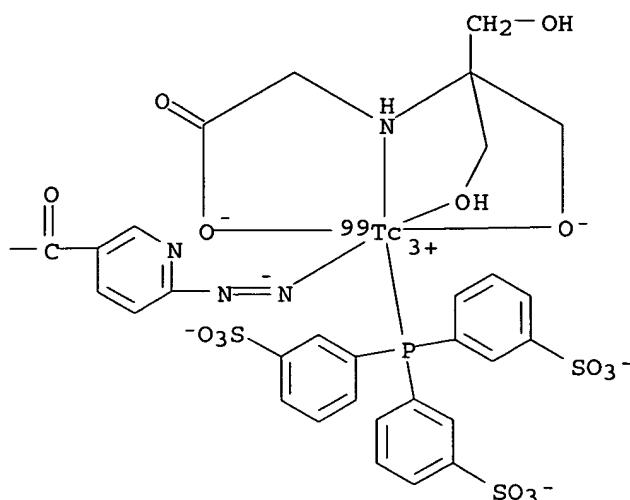
RN 206264-13-3 USPATFULL

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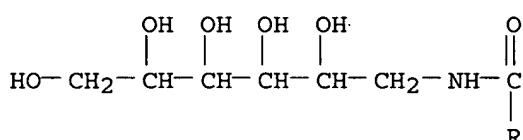
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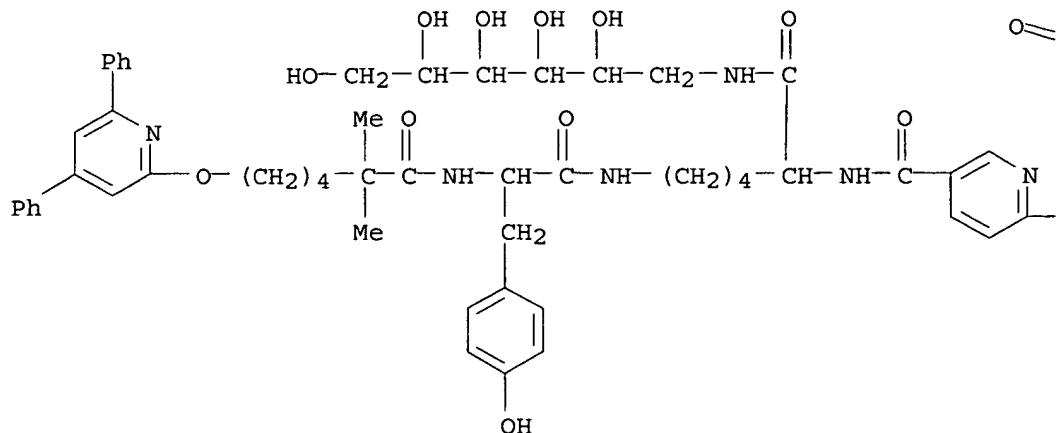
PAGE 2-A

● H^+ ● 3 Na^+

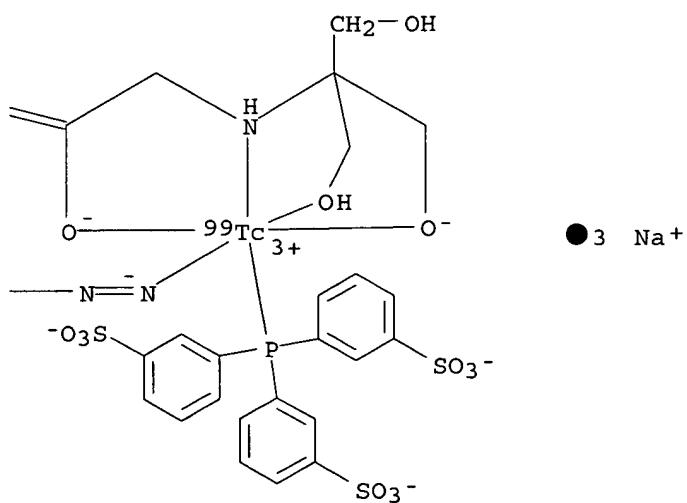
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PAGE 1-A



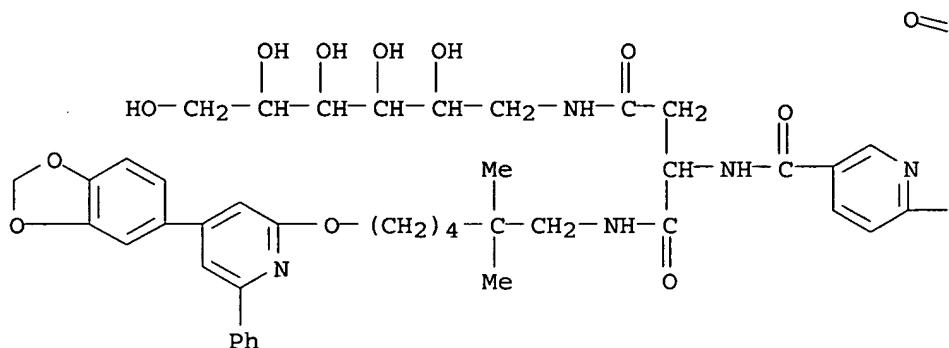
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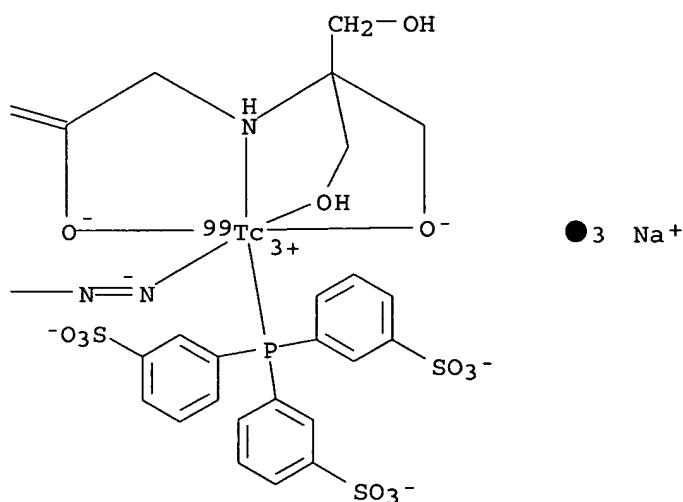
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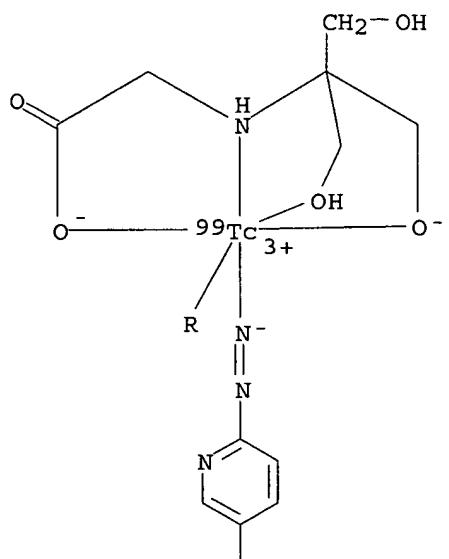
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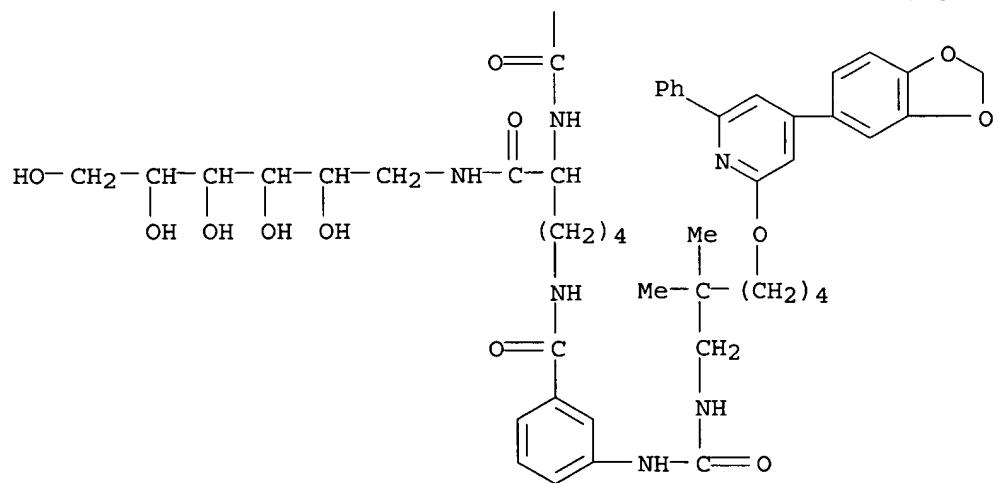
RN 206264-53-1 USPATFULL

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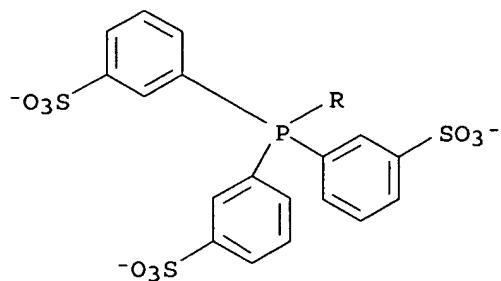
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PAGE 2-A



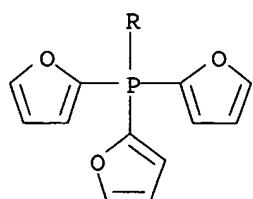
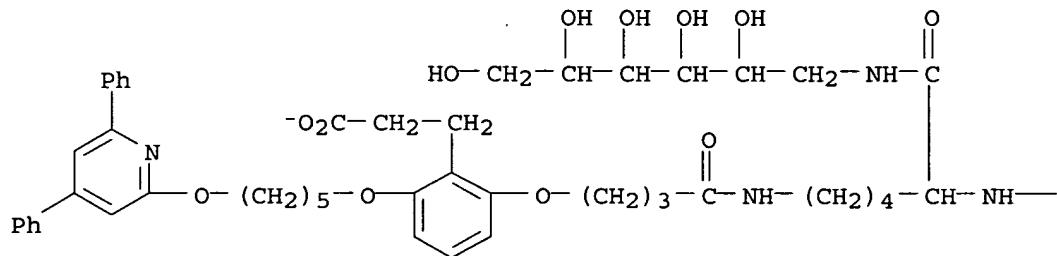
PAGE 3-A

● 3 Na⁺

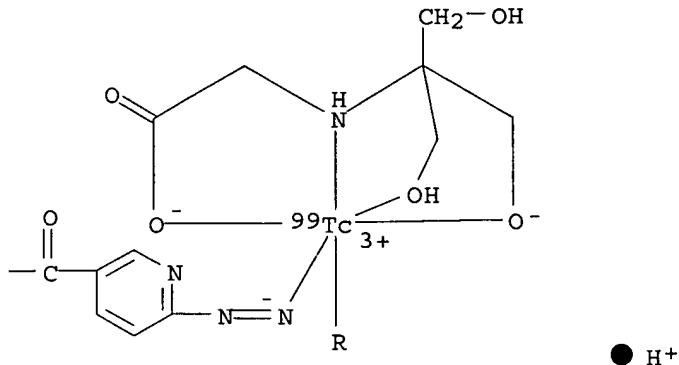
RN 206264-67-7 USPATFULL

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L26 ANSWER 12 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2003:10235 USPATFULL

TITLE: Radiopharmaceuticals for imaging infection and inflammation

INVENTOR(S): Barrett, John A., Groton, MA, UNITED STATES
Cheesman, Edward H., Lunenberg, MA, UNITED STATES
Harris, Thomas D., Salem, NH, UNITED STATES
Liu, Shuang, Chelmsford, MA, UNITED STATES
Rajopadhye, Milind, Westford, MA, UNITED STATES
Sworin, Michael, Tyngsboro, MA, UNITED STATES

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003007927	A1	20030109	<--
APPLICATION INFO.:	US 2002-109374	A1	20020327 (10)	
RELATED APPLN. INFO.:	Continuation of Ser. No. US 1997-943659, filed on 3 Oct 1997, PENDING			

	NUMBER	DATE	
PRIORITY INFORMATION:	US 1996-27955P	19961007 (60)	<--
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	BRISTOL-MYERS SQUIBB PHARMA COMPANY, PATENT DEPARTMENT, P.O. BOX 4000, PRINCETON, NJ, 08543-4000		
NUMBER OF CLAIMS:	31		
EXEMPLARY CLAIM:	1		
LINE COUNT:	9195		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides novel radiopharmaceuticals useful for the diagnosis of infection and inflammation, reagents and kits useful for preparing the radiopharmaceuticals, methods of imaging sites of infection and/or inflammation in a patient, and methods of diagnosing diseases associated with infection or inflammation in patients in need of such diagnosis. The radiopharmaceuticals bind *in vivo* to the leukotriene B4 (LTB4) receptor on the surface of leukocytes which accumulate at the site of infection and inflammation. The reagents provided by this invention are also useful for the treatment of diseases associated with infection and inflammation.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

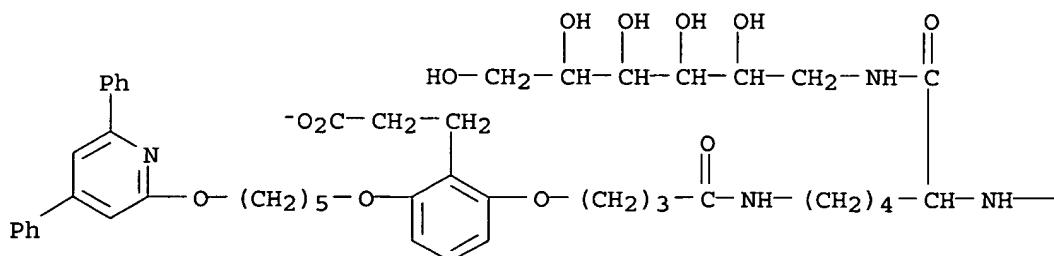
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 206264-13-3P 206264-48-4P, Technetate(3-) -99Tc, [1-deoxy-1-[[N2-[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]-N6-[[6-[(4,6-diphenyl-2-pyridinyl)oxy]-2,2-dimethyl-1-oxohexyl]-L-tyrosyl]-L-lysyl]amino]-D-glucitolato][N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinato(2-)- κ N, κ O][[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium
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(preparation of 99mTc complexes with leukotriene antagonist ligands for imaging and treatment of infection and inflammation)

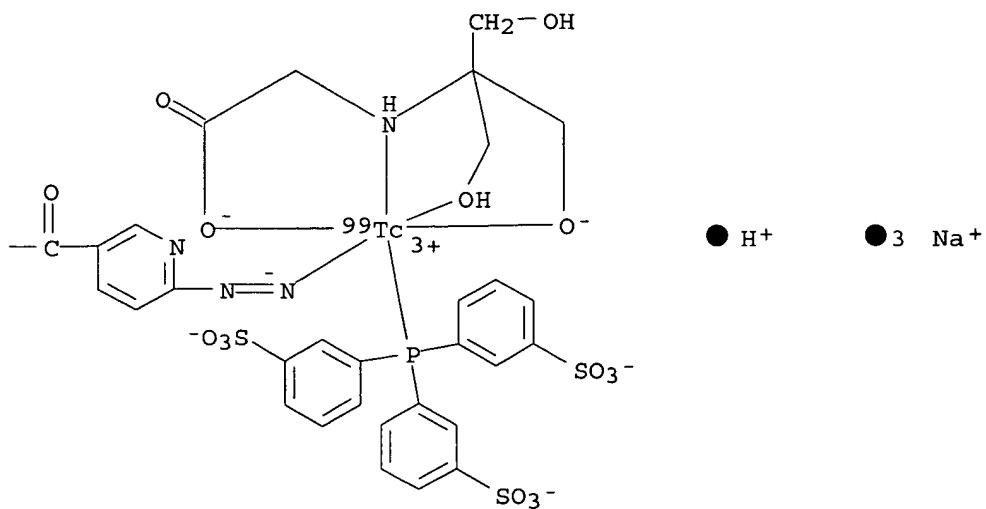
RN 206264-10-0 USPATFULL

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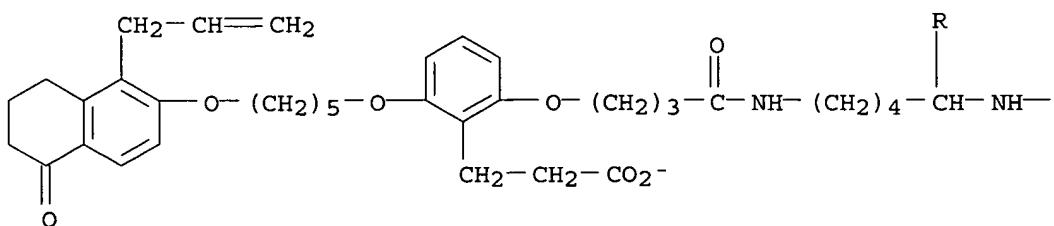
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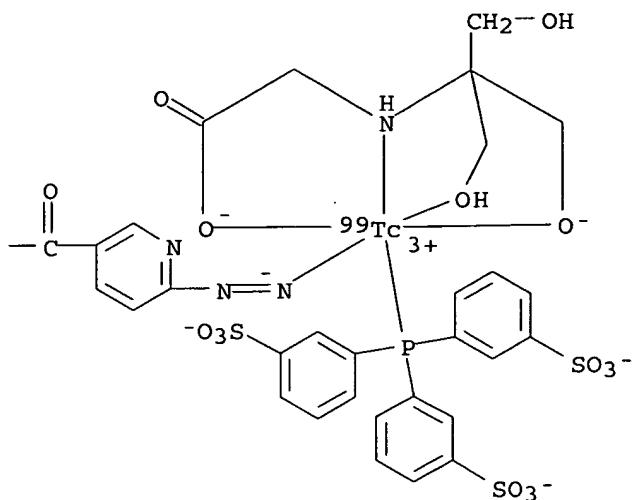
RN 206264-13-3 USPATFULL

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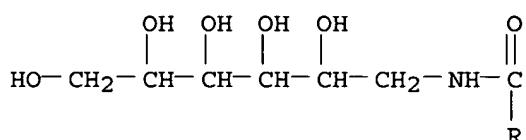
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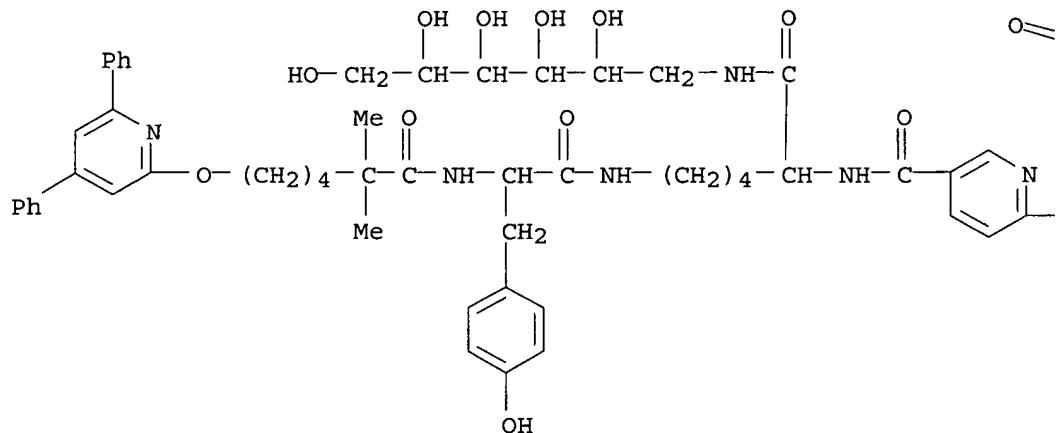
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● H⁺● 3 Na⁺

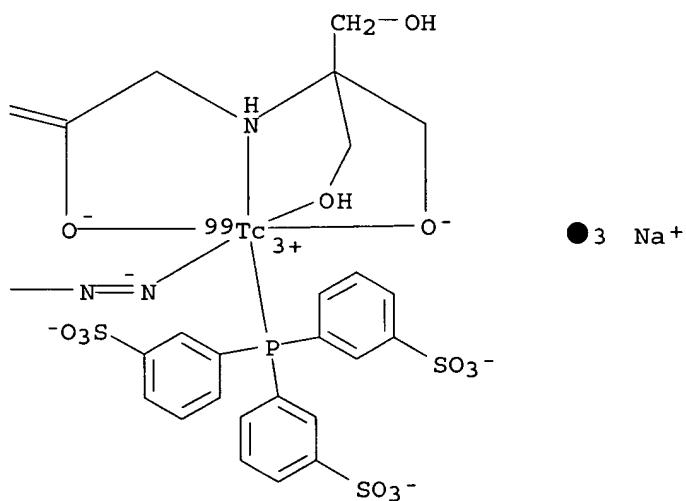
RN 206264-48-4 USPATFULL

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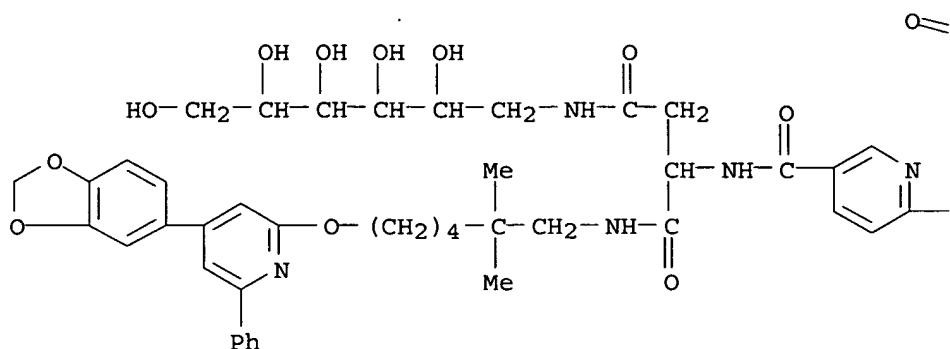
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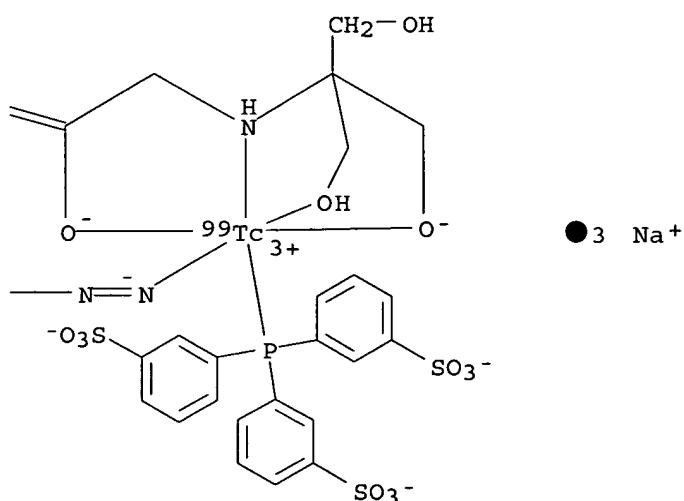
RN 206264-51-9 USPATFULL

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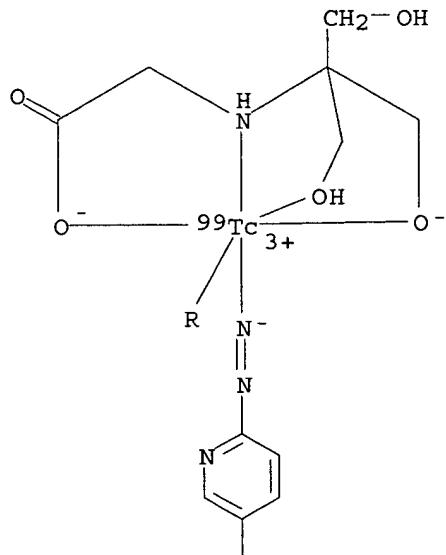
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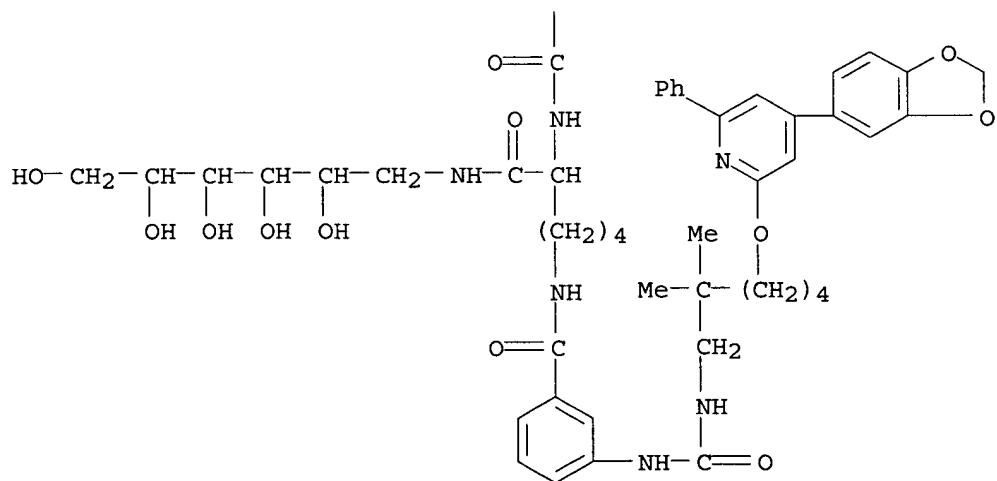
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(CA INDEX NAME)

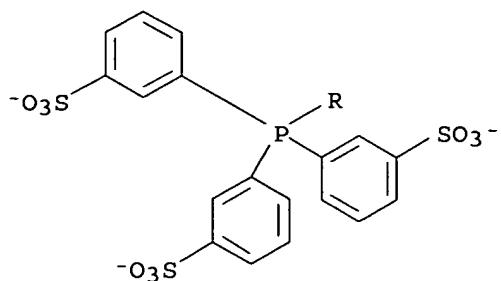
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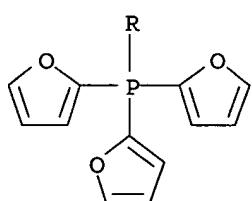
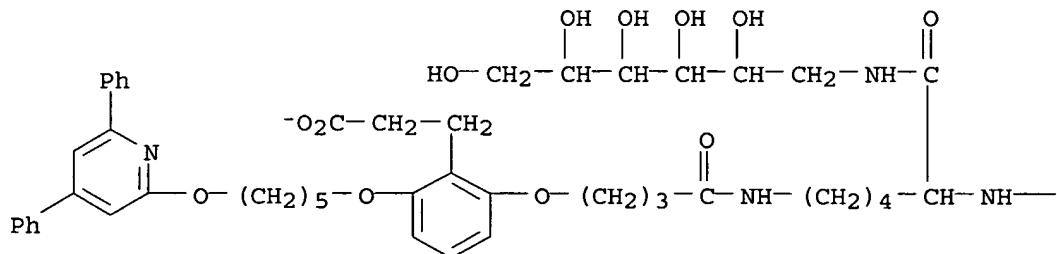
PAGE 3-A

● 3 Na⁺

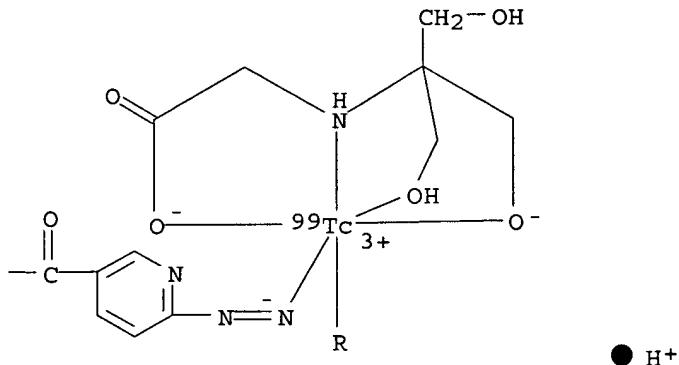
RN 206264-67-7 USPATFULL

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L26 ANSWER 13 OF 17 USPATFULL on STN
 ACCESSION NUMBER: 2003:3016 USPATFULL
 TITLE: Simultaneous dual **isotope** imaging of cardiac perfusion and cardiac inflammation
 INVENTOR(S): Carpenter, Alan P., JR., Carlisle, MA, UNITED STATES

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003003049	A1	20030102	<--
	US 6770259	B2	20040803	
APPLICATION INFO.:	US 2001-2359	A1	20011102 (10)	

	NUMBER	DATE	
PRIORITY INFORMATION:	US 2000-245554P	20001103 (60)	<--
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	BRISTOL-MYERS SQUIBB PHARMA COMPANY, PATENT DEPARTMENT, P.O. BOX 4000, PRINCETON, NJ, 08543-4000		
NUMBER OF CLAIMS:	61		
EXEMPLARY CLAIM:	1		
LINE COUNT:	9537		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides novel diagnostic compositions comprising a **radiolabeled** LTB4 binding agent and a **radiolabeled** perfusion imaging agent, diagnostic kits comprising such compositions, and methods of concurrent imaging in a mammal comprising administering a **radiolabeled** LTB4 binding agent and a **radiolabeled** perfusion imaging agent, and concurrently detecting the **radiolabeled** LTB4 binding agent bound at the LTB4 receptor and the **radiolabeled** perfusion agent.

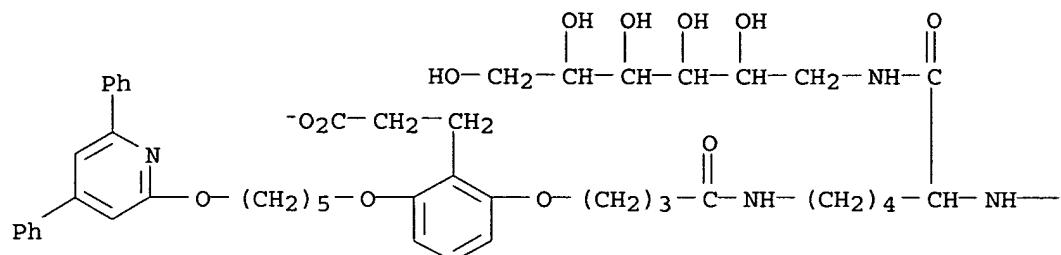
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IT 206264-10-0P 206264-13-3P 206264-48-4P
 206264-51-9P 206264-53-1P 206264-67-7P
 (preparation of 99mTc complexes with leukotriene antagonist ligands for simultaneous dual isotope imaging of perfusion and inflammation)

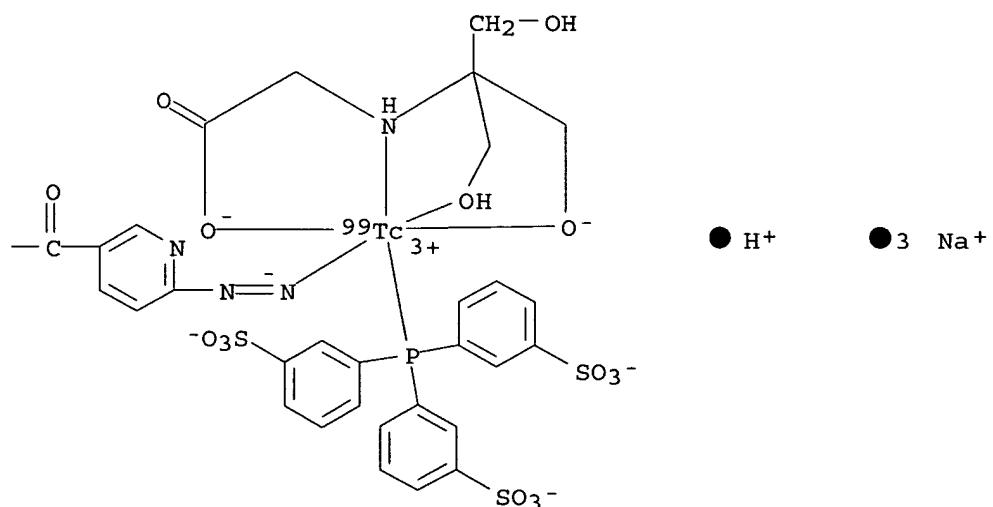
RN 206264-10-0 USPATFULL
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glucitolato(2-)] [[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)], trisodium hydrogen (9CI) (CA INDEX NAME)

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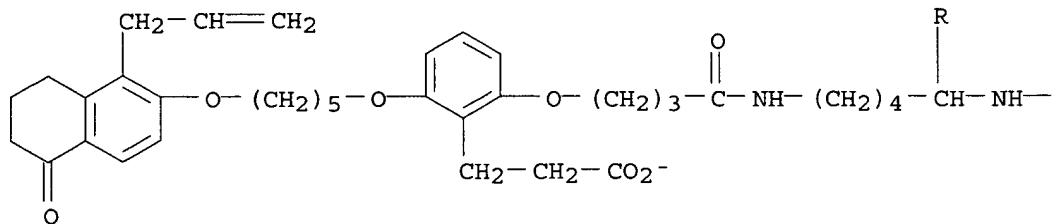
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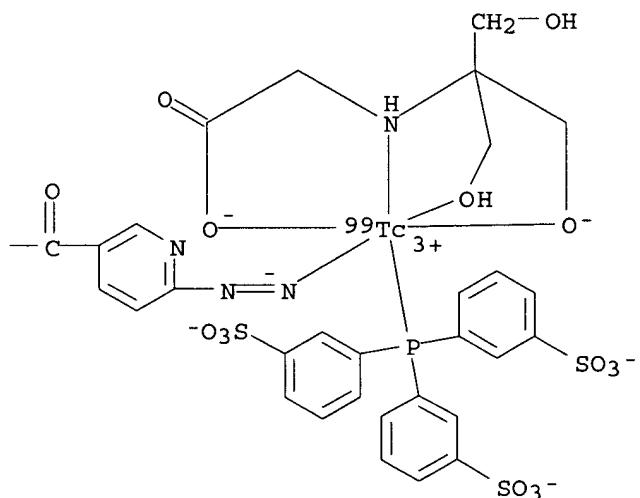
RN 206264-13-3 USPATFULL

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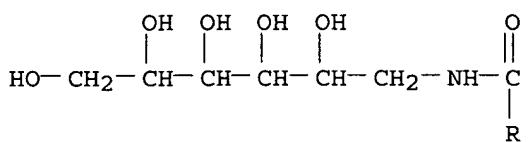
PAGE 1-A



PAGE 1-B



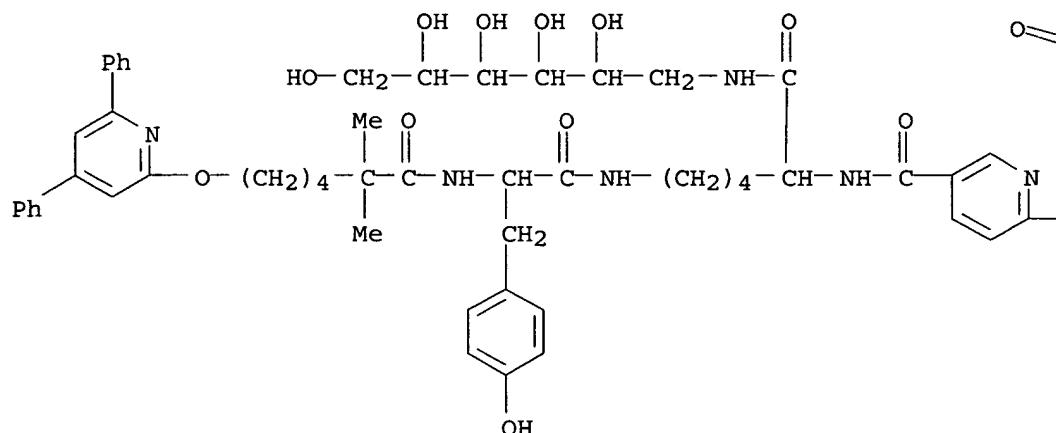
PAGE 2-A

 $\bullet \text{H}^+$ $\bullet 3 \text{ Na}^+$

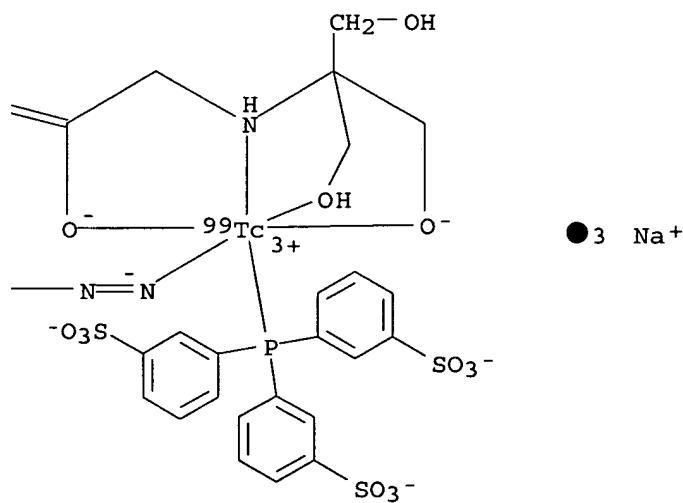
RN 206264-48-4 USPATFULL

CN Technetate(3-) -99Tc, [1-deoxy-1-[[N2-[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]-N6-[N-[6-[(4,6-diphenyl-2-pyridinyl)oxy]-2,2-dimethyl-1-oxohexyl]-L-tyrosyl]-L-lysyl]amino]-D-glucitolato] [N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinato(2-)- κ N, κ O] [[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

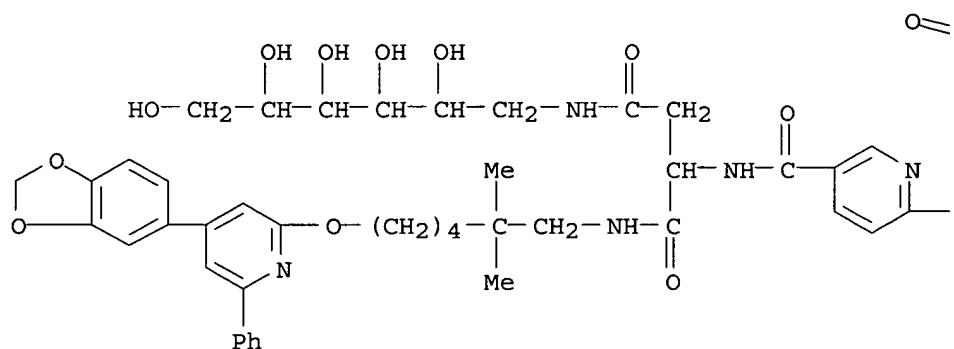


RN 206264-51-9 USPATFULL

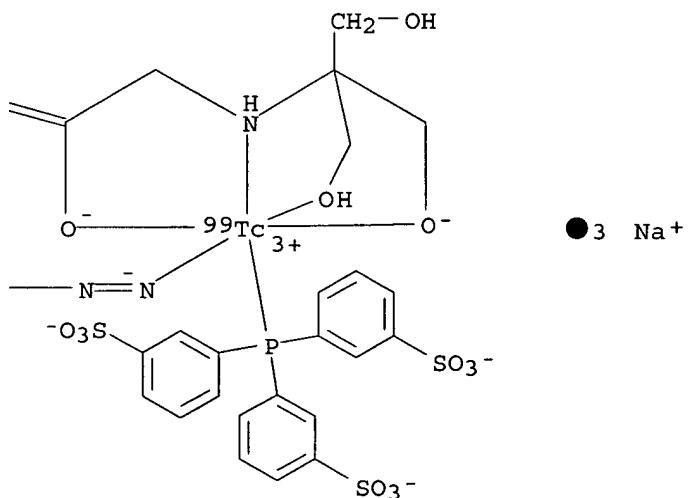
CN Technetate(3-) -99Tc, [1-[[4-[[6-[[4-(1,3-benzodioxol-5-yl)-6-phenyl-2-pyridinyl]oxy]-2,2-dimethylhexyl]amino]-3-[[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]amino]-1,4-dioxobutyl]amino]-1-deoxy-D-glucitolato] [N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinato(2-)-

$\kappa N, \kappa O] [[3, 3', 3'' - (\text{phosphinidyne-}\kappa P)\text{tris}[\text{benzenesulfonato}]](3-)] -, \text{ trisodium (9CI) (CA INDEX NAME)}$

PAGE 1-A



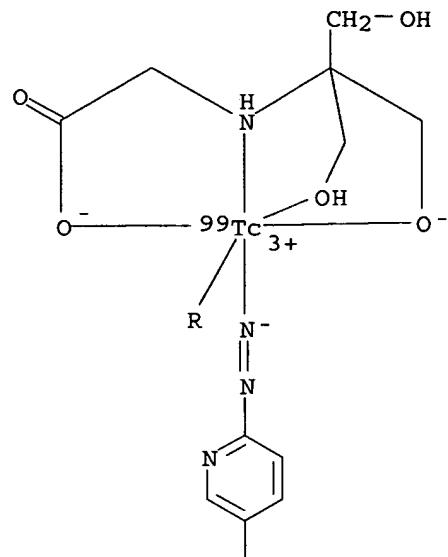
PAGE 1-B



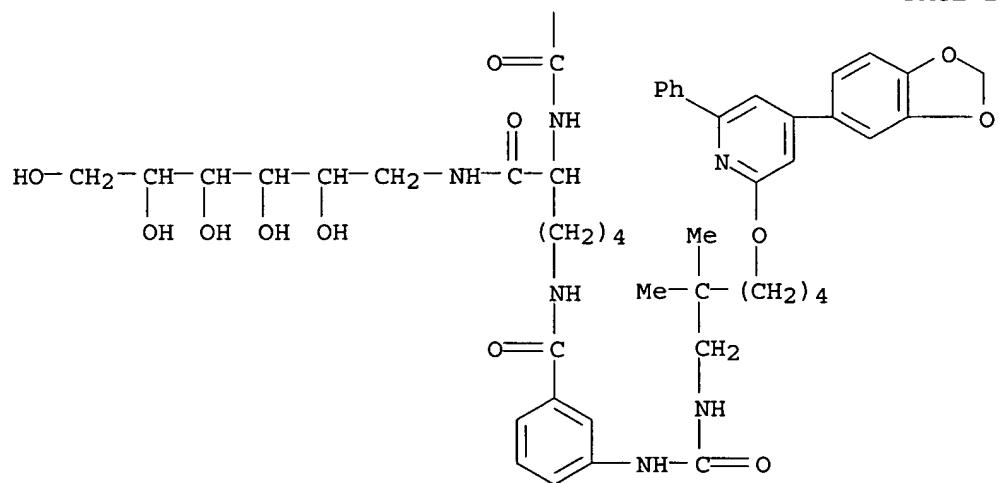
RN 206264-53-1 USPATFULL

CN Technetate(3-) - 99Tc, [1-[[6-[[3-[[6-[[4-(1,3-benzodioxol-5-yl)-6-phenyl-2-pyridinyl]oxy]-2,2-dimethylhexyl]amino]carbonyl]amino]benzoyl]amino]-2-[[6-(diazenyl- κN)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato] [N-[2-hydroxy-1,1-bis[(hydroxymethyl)ethyl]glycinato(2-)- $\kappa N, \kappa O] [[3, 3', 3'' - (\text{phosphinidyne-}\kappa P)\text{tris}[\text{benzenesulfonato}]](3-)] -, \text{ trisodium (9CI) (CA INDEX NAME)}$

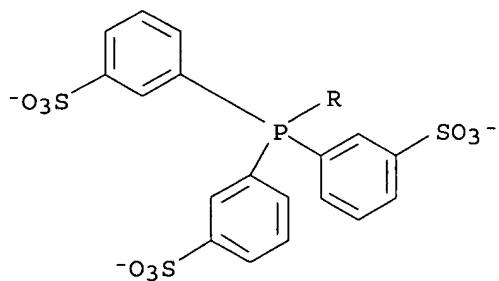
PAGE 1-A



PAGE 2-A



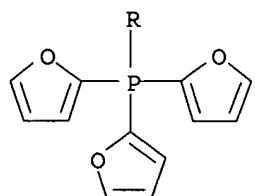
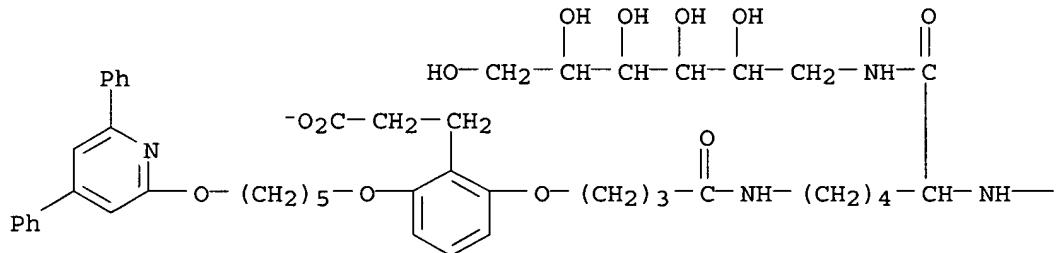
PAGE 3-A

● 3 Na⁺

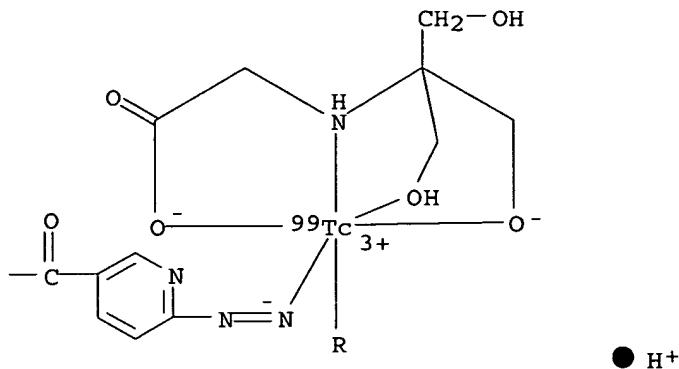
RN 206264-67-7 USPATFULL

CN Technetate(1-) - 99Tc, [1-[[6-[[4-[2-(2-carboxyethyl)-3-[[5-[(4,6-diphenyl-2-pyridinyl)oxy]pentyl]oxy]phenoxy]-1-oxobutyl]amino]-2-[[[6-(diazenyl-κN2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato(2-)][N-[2-hydroxy-1,1-bis([hydroxy-κO)methyl]ethyl]glycinato(2-)-κN,κO] (tri-2-furanylphosphine-κP)-, hydrogen (9CI) (CA INDEX NAME)

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PAGE 1-B



L26 ANSWER 14 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2002:307838 USPATFULL

TITLE: Mass defect labeling for the determination of oligomer sequences

INVENTOR(S): Schneider, Luke V., Half Moon Bay, CA, UNITED STATES
Hall, Michael P., San Carlos, CA, UNITED STATES

Petesch, Robert, Newark, CA, UNITED STATES

PATENT ASSIGNEE(S): Target Discovery, San Carlos, CA, UNITED STATES, 94070
(U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2002172961	A1	20021121	<--
	US 6962818	B2	20051108	
APPLICATION INFO.:	US 2001-35349	A1	20011019 (10)	

	NUMBER	DATE	
PRIORITY INFORMATION:	US 2000-242165P	20001019 (60)	<--
	US 2000-242398P	20001019 (60)	<--

DOCUMENT TYPE: Utility

FILE SEGMENT: APPLICATION

LEGAL REPRESENTATIVE: TOWNSEND AND TOWNSEND AND CREW, LLP, TWO EMBARCADERO CENTER, EIGHTH FLOOR, SAN FRANCISCO, CA, 94111-3834

NUMBER OF CLAIMS: 50

EXEMPLARY CLAIM: 1

NUMBER OF DRAWINGS: 32 Drawing Page(s)

LINE COUNT: 3568

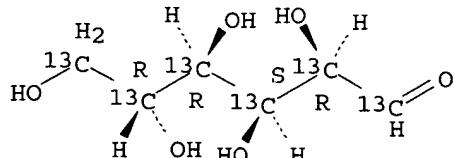
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Mass tagging methods are provided that lead to mass spectrometer detection sensitivities and molecular discriminations that are improved over other methods. In particular the methods are useful for discriminating tagged molecules and fragments of molecules from chemical noise in the mass spectrum. These mass tagging methods are useful for oligomer sequencing, determining the relative abundances of molecules from different samples, and identifying individual molecules or chemical processing steps in combinatorial chemical libraries. The methods provided are useful for the simultaneous analysis of multiple molecules and reaction mixtures by mass spectrometric methods.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 110187-42-3, [13C]6-Glucose
 (detecting metabolites of, in Escherichia coli; polypeptide
 fingerprinting methods and metabolic profiling and apparatus and
 bioinformatics database)
 RN 110187-42-3 USPATFULL
 CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 15 OF 17 USPATFULL on STN
 ACCESSION NUMBER: 2002:167859 USPATFULL
 TITLE: Radiopharmaceuticals for imaging infection and inflammation
 INVENTOR(S): Barrett, John A., Groton, MA, United States
 Cheesman, Edward H., Lunenburg, MA, United States
 Harris, Thomas D., Salem, NH, United States
 Liu, Shuang, Chelmsford, MA, United States
 Rajopadhye, Milind, Westford, MA, United States
 Sworin, Michael, Tyngsboro, MA, United States
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, Princeton, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6416733	B1	20020709	<--
APPLICATION INFO.:	US 1997-943659		19971003 (8)	

	NUMBER	DATE	
PRIORITY INFORMATION:	US 1996-27955P	19961007 (60)	<--
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	GRANTED		
PRIMARY EXAMINER:	Hartley, Michael G.		
LEGAL REPRESENTATIVE:	O'Brien, Maureen P., Dolan, Peter L.		
NUMBER OF CLAIMS:	11		
EXEMPLARY CLAIM:	1		
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)		
LINE COUNT:	8471		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides novel radiopharmaceuticals useful for the diagnosis of infection and inflammation, reagents and kits useful for preparing the radiopharmaceuticals, methods of imaging sites of infection and/or inflammation in a patient, and methods of diagnosing diseases associated with infection or inflammation in patients in need of such diagnosis. The radiopharmaceuticals bind in vivo to the leukotriene B4 (LTB4) receptor on the surface of leukocytes which accumulate at the site of infection and inflammation. The reagents provided by this invention are also useful for the treatment of diseases associated with infection and inflammation.

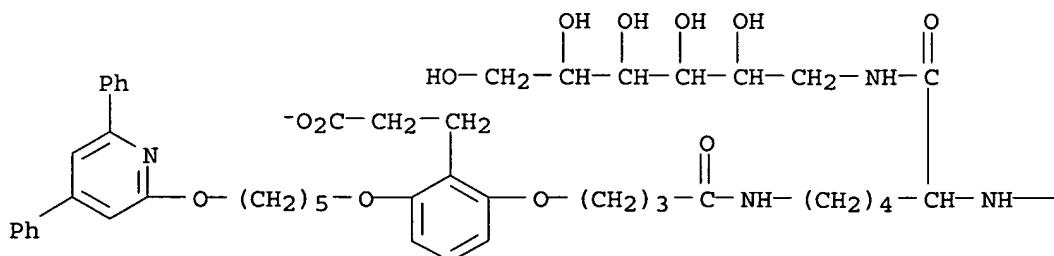
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

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 206264-13-3P 206264-48-4P, Technetate(3-) -99Tc, [1-deoxy-1-[[N2-[[6-(diazetyl- κ N2)-3-pyridinyl]carbonyl]-N6-[[6-[(4,6-diphenyl-2-pyridinyl)oxy]-2,2-dimethyl-1-oxohexyl]-L-tyrosyl]-L-lysyl]amino]-D-glucitolato][N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinato(2-)- κ N, κ O][[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium
 206264-51-9P, Technetate(3-) -99Tc, [1-[[4-[[6-[[4-(1,3-benzodioxol-5-yl)-6-phenyl-2-pyridinyl]oxy]-2,2-dimethylhexyl]amino]-3-[[[6-(diazetyl- κ N2)-3-pyridinyl]carbonyl]amino]-1,4-dioxobutyl]amino]-1-deoxy-D-glucitolato][N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinato(2-)- κ N, κ O][[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium
 206264-53-1P, Technetate(3-) -99Tc, [1-[[6-[[3-[[[[6-[[4-(1,3-benzodioxol-5-yl)-6-phenyl-2-pyridinyl]oxy]-2,2-dimethylhexyl]amino]carbonyl]amino]benzoyl]amino]-2-[[[6-(diazetyl- κ N2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato][N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinat o(2-)- κ N, κ O][[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium 206264-67-7P, Technetate(1-) -99Tc, [1-[[6-[[4-[2-(2-carboxyethyl)-3-[(5-[(4,6-diphenyl-2-pyridinyl)oxy]pentyl)oxy]phenoxy]-1-oxobutyl]amino]-2-[[[6-(diazetyl- κ N2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato(2-)][N-[2-hydroxy-1,1-bis[(hydroxy- κ O)methyl]ethyl]glycinato(2-)- κ N, κ O](tri-2-furanylphosphine- κ P)-, hydrogen
 (preparation of 99mTc complexes with leukotriene antagonist ligands for imaging and treatment of infection and inflammation)

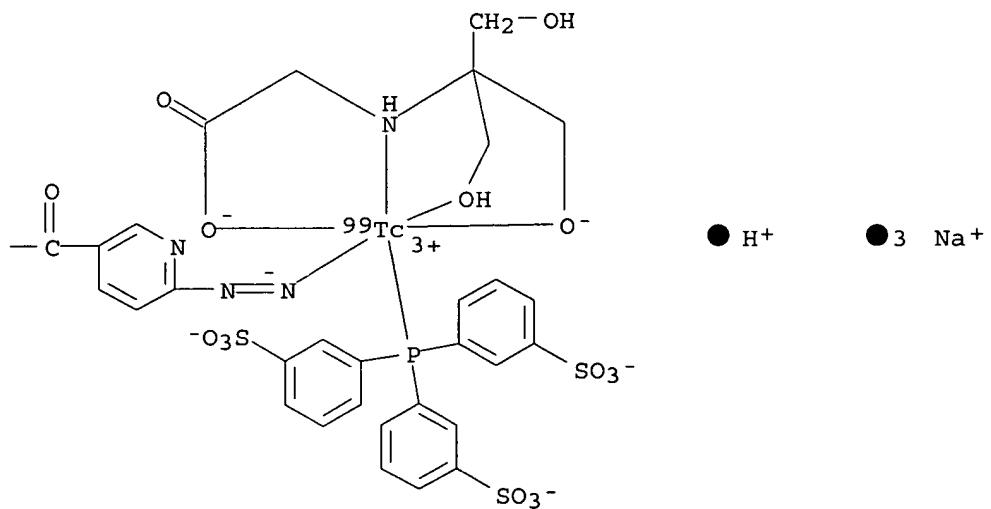
RN 206264-10-0 USPATFULL

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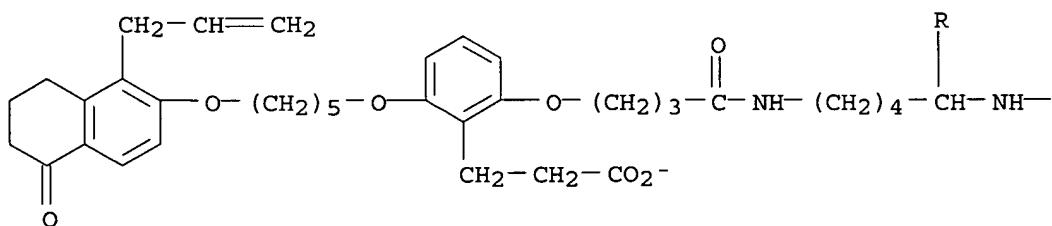
PAGE 1-B



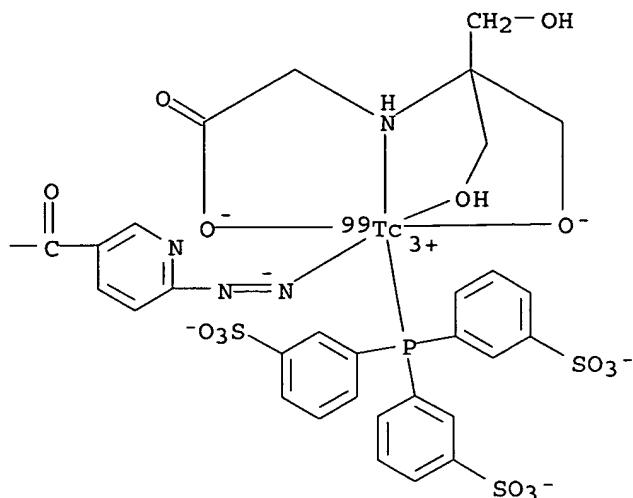
RN 206264-13-3 USPATFULL

CN Technetate (4-) - 99Tc, [1-[[6-[[4-[2-(2-carboxyethyl)-3-[[5-[[5,6,7,8-tetrahydro-5-oxo-1-(2-propenyl)-2-naphthalenyl]oxy]pentyl]oxy]phenoxy]-1-oxobutyl]amino]-2-[[[6-(diazenyl- κ N2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-8-glucitolato(2-)][[3,3',3'''-(phosphinidyne- κ P)tris[benzenesulfonato]](3-)]-, trisodium hydrogen (9CI) (CA INDEX NAME)

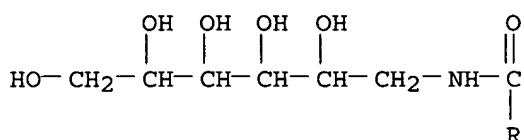
PAGE 1-A



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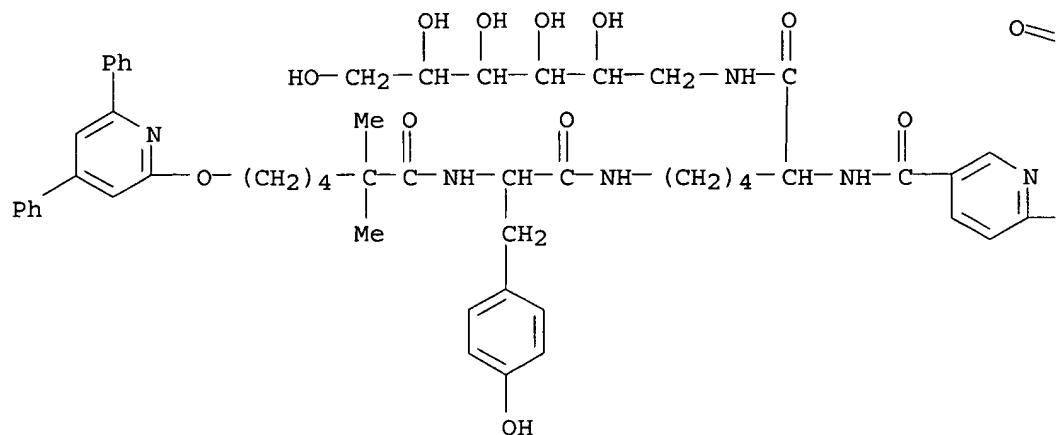


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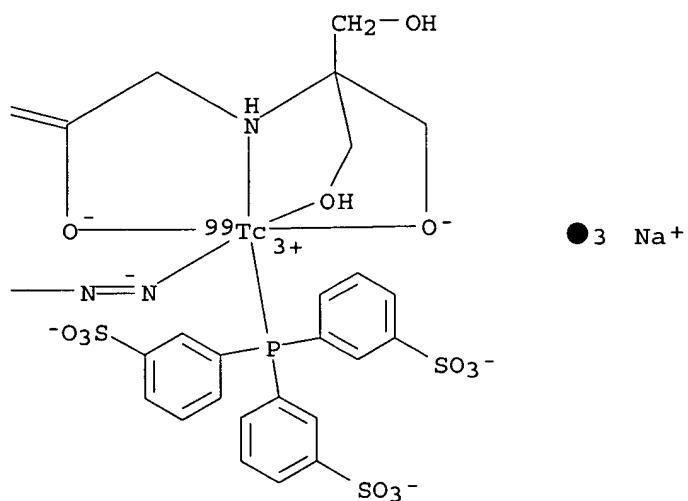
● H⁺● 3 Na⁺

RN 206264-48-4 USPATFULL
 CN Technetate (3-) - 99Tc, [1-deoxy-1-[N2-[[6-(diazenyl-κN2)-3-pyridinyl]carbonyl]-N6-[N-[6-[(4,6-diphenyl-2-pyridinyl)oxy]-2,2-dimethyl-1-oxohexyl]-L-tyrosyl]-L-lysyl]amino]-D-glucitolato] [N-[2-hydroxy-1,1-bis[(hydroxy-κO)methyl]ethyl]glycinato(2-) -κN, κO] [[3,3',3'''-(phosphinidyne-κP)tris[benzenesulfonato]](3-)]-, trisodium (9CI) (CA INDEX NAME)

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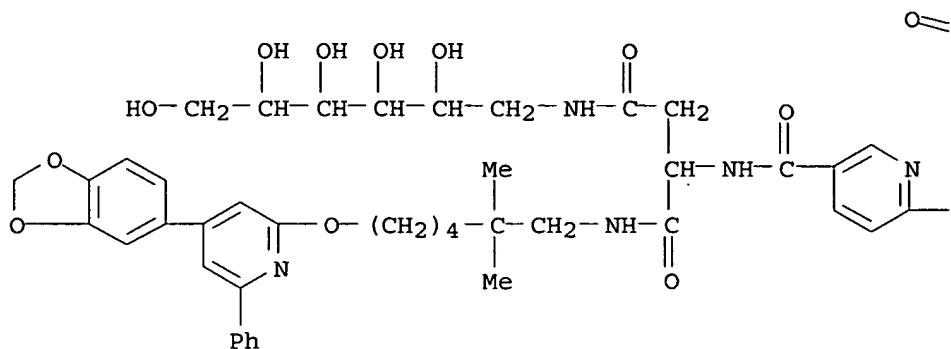
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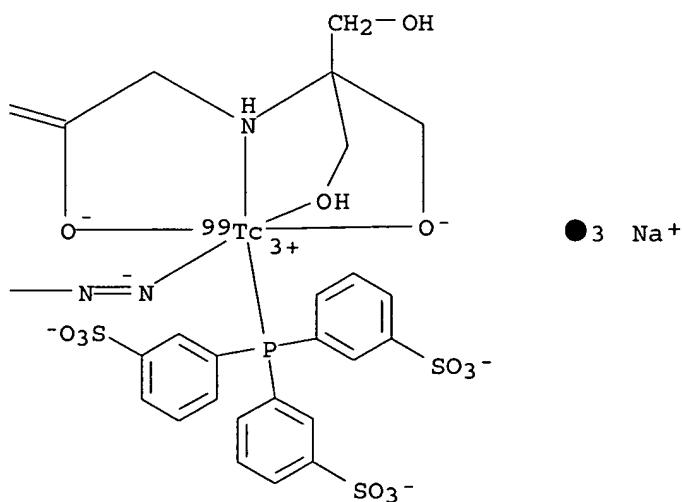
RN 206264-51-9 USPATFULL

CN Technetate(3-) - 99Tc, [1-[[4-[[6-[[4-(1,3-benzodioxol-5-yl)-6-phenyl-2-pyridinyl]oxy]-2,2-dimethylhexyl]amino]-3-[[[6-(diazenyl-κN2)-3-pyridinyl]carbonyl]amino]-1,4-dioxobutyl]amino]-1-deoxy-D-glucitolato] [N-[2-hydroxy-1,1-bis[(hydroxy-κO)methyl]ethyl]glycinato(2-)-κN,κO] [[3,3',3'''-(phosphinidyne-κP)tris[benzenesulfonato]](3-)]-, trisodium (9CI) (CA INDEX NAME)

PAGE 1-A



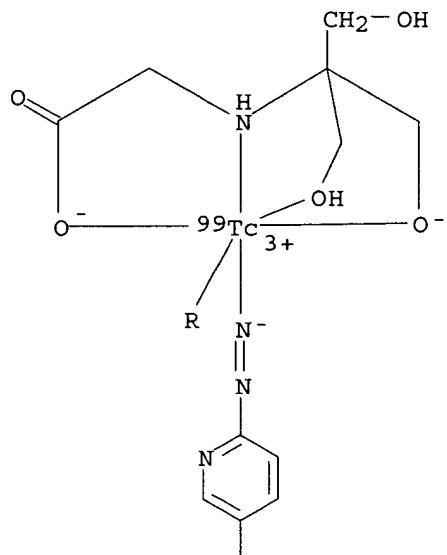
PAGE 1-B



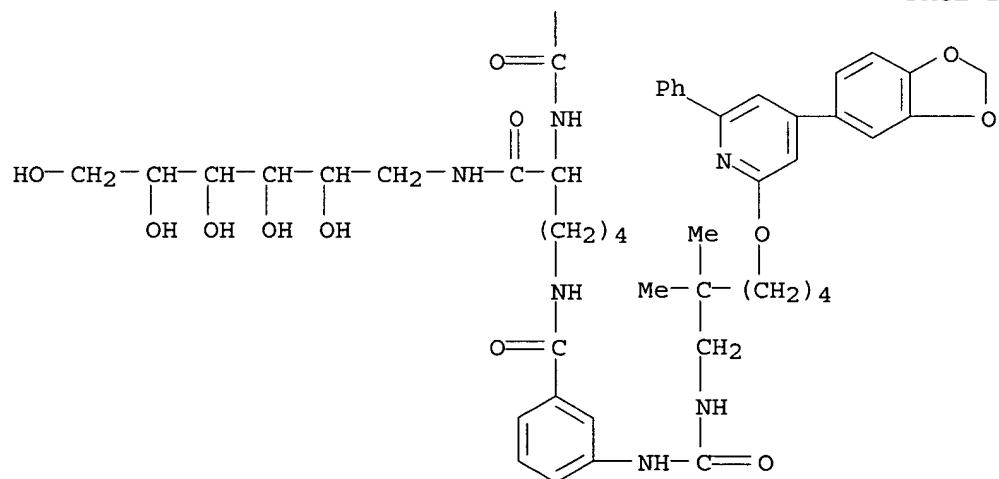
RN 206264-53-1 USPATFULL

CN Technetate (3-) - 99Tc, [1-[6-[[3-[[[6-[4-(1,3-benzodioxol-5-yl)-6-phenyl-2-pyridinyl]oxy]-2,2-dimethylhexyl]amino]carbonyl]amino]benzoyl]amino]-2-[[[6-(diazenyl-κN2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato] [N-[2-hydroxy-1,1-bis[(hydroxy-κO)methyl]ethyl]glycinato(2-)-κN, κO] [[3,3',3'''-(phosphinidyne-κP)tris[benzenesulfonato]](3-)]-, trisodium (9CI) (CA INDEX NAME)

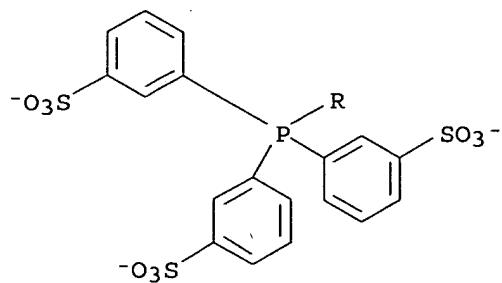
PAGE 1-A



PAGE 2-A



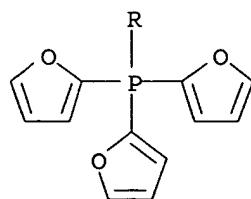
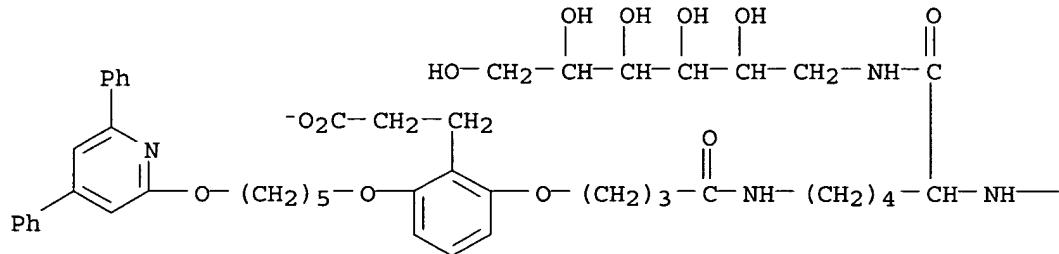
PAGE 3-A

● 3 Na⁺

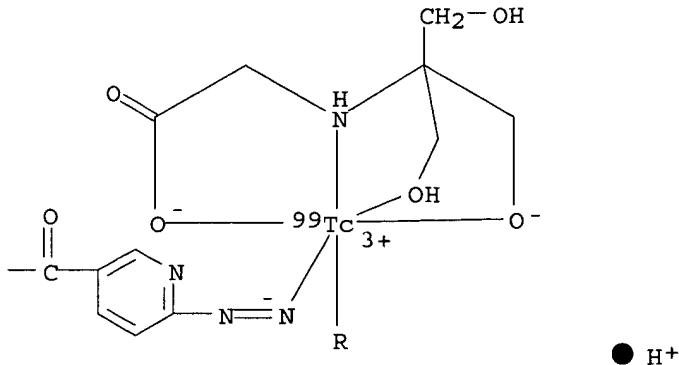
RN 206264-67-7 USPATFULL

CN Technetate(1-) - 99Tc, [1-[[6-[[4-[2-(2-carboxyethyl)-3-[[5-[(4,6-diphenyl-2-pyridinyl)oxy]pentyl]oxy]phenoxy]-1-oxobutyl]amino]-2-[[6-(diazenyl-κN2)-3-pyridinyl]carbonyl]amino]-1-oxohexyl]amino]-1-deoxy-D-glucitolato(2-)] [N-[2-hydroxy-1,1-bis[(hydroxy-κO)methyl]ethyl]glycinato(2-)-κN, κO] (tri-2-furanylphosphine-κP)-, hydrogen (9CI) (CA INDEX NAME)

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PAGE 1-B



L26 ANSWER 16 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2000:1689 USPATFULL

TITLE: Methods for measuring cellular proliferation and destruction rates in vitro and in vivo

INVENTOR(S): Hellerstein, Marc K., Kensington, CA, United States

PATENT ASSIGNEE(S): The Regents of the University of California, Oakland, CA, United States (U.S. corporation)

NUMBER KIND DATE

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PATENT INFORMATION: US 6010846 20000104 <--
 APPLICATION INFO.: US 1998-75309 19980508 (9)
 RELATED APPLN. INFO.: Continuation-in-part of Ser. No. US 1997-857007, filed on 15 May 1997, now patented, Pat. No. US 5910403

DOCUMENT TYPE: Utility

FILE SEGMENT: Granted

PRIMARY EXAMINER: Gitomer, Ralph

LEGAL REPRESENTATIVE: Townsend and Townsend and Crew LLP

NUMBER OF CLAIMS: 24

EXEMPLARY CLAIM: 1

NUMBER OF DRAWINGS: 29 Drawing Figure(s); 17 Drawing Page(s)

LINE COUNT: 2901

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to methods for measuring the proliferation and destruction rates of cells by measuring deoxyribonucleic acid (DNA) synthesis and/or destruction. In particular, the methods utilize non-radioactive stable isotope labels to endogenously label DNA synthesized through the de novo nucleotide synthesis pathway in a cell. The amount of label incorporated in the DNA is measured as an indication of cellular proliferation. The decay of labeled DNA over time is measured as an indication of cellular destruction. Such methods do not involve radioactivity or potentially toxic metabolites, and are suitable for use both in vitro and in vivo. Therefore, the invention is useful for measuring cellular proliferation or cellular destruction rates in humans for the diagnosis, prevention, or management of a variety of disease conditions in which cellular proliferation or cellular destruction is involved. The invention also provides methods for measuring proliferation or destruction of T cells in a subject infected with human immunodeficiency virus (HIV) and methods of screening an agent for a capacity to induce or inhibit cellular proliferation or

destruction. In addition, the invention provides methods for measuring cellular proliferation in a proliferating population which utilize both radioactive isotope labels and stable isotopes to endogenously label DNA through the de novo nucleotide synthesis pathway.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

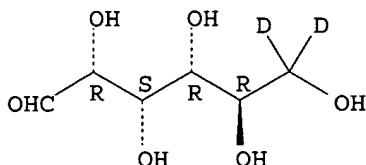
IT 18991-62-3, D-Glucose-6,6-C-d2 70849-17-1,
D-Glucose-2-13C 110187-42-3, D-Glucose-13C6

(measuring cellular proliferation and destruction rates in vitro and in vivo using isotope labels on DNA)

RN 18991-62-3 USPATFULL

CN D-Glucose-6,6-C-d2 (9CI) (CA INDEX NAME)

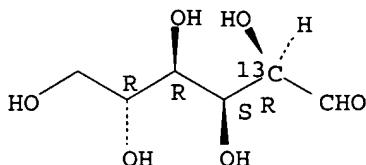
Absolute stereochemistry.



RN 70849-17-1 USPATFULL

CN D-Glucose-2-13C (9CI) (CA INDEX NAME)

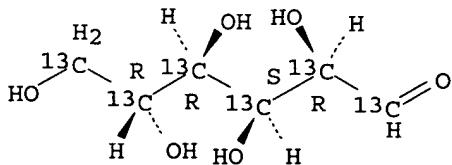
Absolute stereochemistry.



RN 110187-42-3 USPATFULL

CN D-Glucose-13C6 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 17 OF 17 USPATFULL on STN

ACCESSION NUMBER: 1999:1210 USPATFULL

TITLE: Hydroxymethyl phosphine compounds for use as diagnostic and therapeutic pharmaceuticals and method of making same

INVENTOR(S): Katti, Kattesh V., Columbia, MO, United States
Karra, Srinivasa Rao, Columbia, MO, United States
Berning, Douglas E., Columbia, MO, United States
Smith, C. Jeffrey, Columbia, MO, United States

PATENT ASSIGNEE(S): Volkert, Wynn A., Columbia, MO, United States
 Ketring, Alan R., Columbia, MO, United States
 The Curators of the University of Missouri, Columbia,
 MO, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5855867	19990105	<--
APPLICATION INFO.:	US 1997-818080	19970314 (8)	
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1995-412470, filed on 29 Mar 1995, now abandoned		
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Hollinden, Gary E.		
ASSISTANT EXAMINER:	Hartley, Michael G.		
LEGAL REPRESENTATIVE:	Kohn & Associates		
NUMBER OF CLAIMS:	19		
EXEMPLARY CLAIM:	1		
NUMBER OF DRAWINGS:	21 Drawing Figure(s); 9 Drawing Page(s)		
LINE COUNT:	2848		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A compound and method of making a compound for use as a diagnostic or therapeutic pharmaceutical comprises at least one functionalized hydroxyalkyl phosphine donor group and one or more sulfur or nitrogen donor and a metal combined with the ligand.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

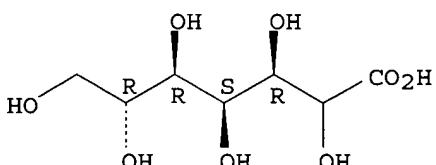
IT 68128-55-2

(reaction; hydroxymethyl phosphine compds., and preparation thereof, for use as diagnostic and therapeutic pharmaceuticals)

RN 68128-55-2 USPATFULL

CN D-gluco-Heptonic acid, technetium-99Tc salt, (2 ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● x 99Tc (x)